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Spectroscopic Constants for Selected Homonuclear Diatomic Molecules

Volume II. K Through Z

S. N. SUCHARD and J. E. MELZER
Aerophysics Laboratory
Laboratory Operations
The Aerospace Corporation
El Segundo, Calif. 90245

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) Spectroscopic information relevant to homonuclear diatomic molecules has been collected and is presented. This information includes not only the molecular band systems, but also Frank-Condon factors, oscillator strengths, potential energy curves, and reactive branching ratios, where available. The information is arranged alphabetically by molecule in two volumes. This, the second volume, covers K through Z.		

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19. KEY WORDS (Continued)

Molecular Band System
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Reaction Rate
Spectroscopic Constant
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20. ABSTRACT (Continued)

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PREFACE

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I. INTRODUCTION

A complete discussion of the purpose, organization, and notation used in this compilation and comments on the availability of spectroscopic information are presented in Volume I of this report. The only intent here is to outline the text of Volume I, to which the reader is referred.

Generally, the information on the alphabetically arranged molecules is broken into five separate sections: viz., methods of production and experimental technique, band systems, spectroscopic constants, perturbations and general information, and bibliography. These are described briefly.

METHODS OF PRODUCTION AND EXPERIMENTAL TECHNIQUE

Sources for the production of the molecule and techniques for study are presented.

BAND SYSTEMS

A general description is given of the molecular transition of each system or group. The system is analyzed in detail.

SPECTROSCOPIC CONSTANTS

The molecular constants that totally define the electronic states of the molecule are given. The bulk of the dissociation energy information is taken from Gaydon (Ref. 7 in Vol I); other sources are so noted.

PERTURBATIONS AND GENERAL INFORMATION

All other information deemed useful to the complete understanding of the molecule is included here.

BIBLIOGRAPHY

The referencing system (after Suchard, Ref. 4 in Vol I) is made up of two numbers: first, the year of publication; second, the running count of references cited for each molecule.

Also presented in Volume I is a section "Notation and Notational Conversion Formulas." Formulas are given for such molecular properties as total energy of a given state of the molecule T , electronic energy T_e , vibrational energy G , and rotational energy F . Nomenclature for other molecular constants reported is also given.

MOLECULE	VIBRA- TIONAL CONSTANTS	ROTA- TIONAL CONSTANTS	VIBRA- TIONAL LEVEL DISTRIBU- TIONS	DISSO- CIATION ENERGY	LIFE- TIMES	FRANCK- CONDON FACTORS	BRANCH- ING RATIOS	QUENCH- ING	LASER ACTION OBSERVED	
									VIBRA- TIONAL	ELEC- TRONIC
Ac ₂										
Ag ₂	X			X						
Al ₂	X	X		X						
Am ₂										
Ar ₂	P	P		X						X
As ₂	X	X		X		P		P		
At ₂										
Au ₂	X	X		X		P				
B ₂	X	X		X						
Ba ₂										
Be ₂				P						
Bi ₂	X	P		X						
Bk ₂										
Br ₂	X	X	P	X	P	X		P		
C ₂	X	X	P	X	X					
Ca ₂	P	P		X						
Cd ₂										
Ce ₂				X						
Cf ₂										
Cl ₂	X	P		X		P		P		
Cm ₂										
Co ₂				X						
Cr ₂				X						
Cs ₂	X			X	P					
X=SUBSTANTIAL INFORMATION; P=SKETCHY INFORMATION; NO NOTATION=NO INFORMATION										

Chart II-1

MOLECULE	VIBRA- TIONAL CONSTANTS	ROTA- TIONAL CONSTANTS	VIBRA- TIONAL LEVEL DISTRIBU- TIONS	DISSO- CIATION ENERGY	LIFE- TIMES	FRANCK- CONDON FACTORS	BRANCH- ING RATIOS	QUENCH- ING	LASER ACTION OBSERVED	
									VIBRA- TIONAL	ELEC- TRONIC
Cu ₂	X	P		X		P				
Dy ₂				X						
Er ₂				X						
Es ₂										
Eu ₂				X						
F ₂	P	P		X						
Fe ₂				X						
Fm ₂										
Fr ₂										
Ga ₂				X						
Gd ₂				X						
Ge ₂				X						
H ₂	X	X	P	X	X	X		X		X
He ₂	X	X		X						X
Hf ₂										
Hg ₂				X						
Ho ₂										
I ₂	X	X	P	X	P	X		X		X
In ₂	X			P						
Ir ₂										
K ₂	X	P		X	P					
Kr ₂	X	P		X						X
La ₂	P			X						
Li ₂	X	X		X	P					
X=SUBSTANTIAL INFORMATION; P=SKETCHY INFORMATION; NO NOTATION=NO INFORMATION										

Chart II-2

MOLECULE	VIBRA- TIONAL CONSTANTS	ROTA- TIONAL CONSTANTS	VIBRA- TIONAL LEVEL DISTRIBU- TIONS	DISSO- CIATION ENERGY	LIFE- TIMES	FRANCK- CONDON FACTORS	BRANCH- ING RATIOS	QUENCH- ING	LASER ACTION OBSERVED	
									VIBRA- TIONAL	ELEC- TRONIC
Lu ₂										
Md ₂										
Mg ₂	X	X		X		X				
Mn ₂				X						
Mo ₂										
N ₂	X	X	P	X	X	X		X		X
Na ₂	X	X		X	P	P				
Nb ₂										
Nd ₂				X						
Ne ₂	P	P		X	P					
Ni ₂				X						
No ₂										
Np ₂										
O ₂	X	X	P	X	X	X		X		
Os ₂										
P ₂	X	P		X				P		
Pa ₂										
Pb ₂	X			X						
Pd ₂				X						
Pm ₂										
Po ₂	X			X						
Pr ₂				X						
Pt ₂										
Pu ₂										
X=SUBSTANTIAL INFORMATION; P=SKETCHY INFORMATION; NO NOTATION=NO INFORMATION										

Chart II-3

MOLECULE	VIBRA- TIONAL CONSTANTS	ROTA- TIONAL CONSTANTS	VIBRA- TIONAL LEVEL DISTRIBUTIONS	DISSO- CIATION ENERGY	LIFE- TIMES	FRANCK- CONDON FACTORS	BRANCH- ING RATIOS	QUENCH- ING	LASER ACTION OBSERVED	
									VIBRA- TIONAL	ELEC- TRONIC
Ra ₂										
Rb ₂	X			X	P			P		
Re ₂										
Rh ₂										
Rn ₂										
Ru ₂										
S ₂	X	X		X	P			P		
Sb ₂	X	P		X				P		
Sc ₂				X						
Se ₂	X	X		X				P		
Si ₂	X	X		X				P		
Sm ₂				X						
Sn ₂				X						
Sr ₂										
Ta ₂										
Tb ₂				X						
Tc ₂										
Te ₂	X	X		X		X				
Th ₂				X						
Ti ₂				X						
Tl ₂				X						
Tm ₂				X						
U ₂				X						
V ₂				X						
X=SUBSTANTIAL INFORMATION; P=SKETCHY INFORMATION; NO NOTATION=NO INFORMATION										

Chart II-4

MOLECULE	VIBRA- TIONAL CONSTANTS	ROTA- TIONAL CONSTANTS	VIBRA- TIONAL LEVEL DISTRIBUTIONS	DISSO- CIATION ENERGY	LIFE- TIMES	FRANCK- CONDON FACTORS	BRANCH- ING RATIOS	QUENCH- ING	LASER ACTION OBSERVED	
									VIBRA- TIONAL	ELEC- TRONIC
W ₂										
Xe ₂	P			X	P			P		X
Y ₂				X						
Yb ₂				X						
Zn ₂				P						
Zr ₂										
X=SUBSTANTIAL INFORMATION; P=SKETCHY INFORMATION; NO NOTATION=NO INFORMATION										

Chart II-5

Methods of Production and Experimental Technique

Absorption.

Emission from a heat pipe, laser fluorescence.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$A^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$	Heat Pipe	8850-7700	R			(71.47, 30.10)
	II	$B^1\Pi_u \leftarrow X^1\Sigma_g^+$	Absorption, laser fluores- cence	6950-6250	R	6583.2(0, 2) 6544.0(0, 1) 6473.6(1, 0)		(68.39, 32.15, 31.12)
	III	$C^1\Pi_u \leftarrow X^1\Sigma_g^+$	Absorption	4510-4220	R	4343.5(1, 0)		(61.32, 48.29)
	IV	$D(^1\Pi_u) \leftarrow X^1\Sigma_g^+$	Absorption	4160-3940	R	4082.7(1, 2)		(48.29)
	V	$E(^1\Pi_u) \leftarrow X^1\Sigma_g^+$	Absorption	3925-3700	R	3797.6(2, 3) 3793.7(1, 2)		(50.31)
	VI	$F \leftarrow X^1\Sigma_g^+$	Absorption	3700-3600	R			(37.20, 37.19)
	VII	$G \leftarrow X^1\Sigma_g^+$	Absorption	3600-3480	R			(37.19)

Molecule K₂

I. $A^1\Sigma_u^+ \rightleftharpoons X^1\Sigma_g^+$ SystemMost characteristic bands, λ (30.10):

(v', v'')	(0, 3)	(0, 2)	(1, 2)	(0, 1)	(0, 0)	(1, 0)	(2, 0)
λ	8773.15	8702.00	8651.79	8634.43	8566.30	8515.70	8468.23

II. $B^1\Pi_u \rightleftharpoons X^1\Sigma_g^+$ SystemMost intense band heads, λ (Intensity) (32.15, 31.12):

v', v''	(0, 2)	(0, 1)	(1, 1)	(1, 0)	(2, 0)
λ	6583.19	6544.00	6512.19	6473.58	6443.00
(Intensity)	9	8	5	10	8

III. $C^1\Pi_u \rightleftharpoons X^1\Sigma_g^+$ SystemMost intense band heads, λ (Intensity) (61.32, 48.29):

v', v''	(0, 0)	(1, 0)	(2, 0)	(3, 0)	(4, 0)
λ	4355.1	4343.5	4332.3	4320.9	4310.0
(Intensity)	8	10	7	7	7

IV. $D(^1\Pi_u) \leftarrow X^1\Sigma_g^+$ SystemPossibly two independent systems, λ (Intensity) (27.20, 37.19):

v', v''	0	1	2	3	4	5
0			4092.3(8)	4107.3(7)	4122.7(6)	
1		4067.0(8)	4082.7(10)	4097.4(7)	4112.8(8)	
2				4087.5(6)	4103.0(6)	
3	4033.5(6)			4078.2(6)		4108.6(6)
4	4024.9(6)					

V. $E(^1\Pi_u) \leftarrow X^1\Sigma_g^+$ System

Most intense band heads, λ (Intensity) (50.31):

v', v''	0	1	2	3
0				
1			3793.7(10)	3806.2(7)
2		3771.5(8)	3784.4(7)	3797.6(10)
3		3762.8(7)	3776.0(7)	3789.2(7)
4				
5	3733.8(7)	3746.6(7)		
6		3738.1(7)		

VI. $F \leftarrow X^1\Sigma_g^+$ System

Most intense band heads, analysis uncertain, λ (37.20, 37.19):

v', v''	0	1	2	3
0		3639.5	3651.7	
1		3631.6	3643.4	
2	3611.2	3623.5	3635.3	3647.3
3	3603.2			

VII. $G \leftarrow X^1\Sigma_g^+$ System

Most intense band heads, λ (Intensity) (37.19):

(v', v'')	(0, 2)	(1, 2)	(2, 2)	(3, 2)	(4, 2)	(3, 1)	(4, 1)
λ	3583.7	3575.6	3567.6	3559.9	3553.4	3548.6	3541.1
(Intensity)	4	4	4	3	4	3	3

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e \omega_e$	$B_e \times 10^2$	$\alpha_e \times 10^4$	$D_e \times 10^8$	r_e	Remarks	Bibliography
G	28091	64.9	0.05						(37.19)
F	27571	62.2	0.24						(37.19)
$E(^1\Pi_u)$	26493.0	60.6	0.15						(50.31)
$D(^1\Pi_u)$	24627.7	61.6	0.90					(a)	(48.29)
$C^1\Pi_u$	22969.7	61.48	0.14	4.404	1.10		4.43		(61.32, 50.31)
$B^1\Pi_u$	15376.4	92.021	0.2829	5.6743	1.65	8.63	4.23	(b)	(68.39, 32.15, 31.13)
$A^1\Sigma_u^+$	11682.6	69.09	0.153						(30.10)
$X^1\Sigma_g^+$	0	92.64		5.622	2.19	8.28	3.92	(c)	(61.32, 48.29)

(a) $y_{ee}^w = 0.001$, $z_{ee}^w = -0.0003$; (b) $y_{ee}^w = -0.002055$, $\gamma_e = -7.2 \times 10^{-6}$, $\delta_e = 1.5 \times 10^{-7}$, $\beta = -7.4 \times 10^{-10}$;
(c) $\beta = -8.3 \times 10^{-11}$

Dissociation energy = 0.51 ± 0.05 eV, 11.8 kcal/mole, 4114 cm^{-1} .

Perturbations and General InformationRadiative lifetime of B¹Π_u state (70.44, 70.41):

$$\tau(B^1\Pi_u) = 9.65 \pm 0.3 \text{ nsec.}$$

Absolute absorption cross sections (68.37, 66.35).

Potential energy curves, RKR potentials (69.40):

	State	v	U(cm ⁻¹)	r _{min} (Å)	r _{max} (Å)
T _e = 0.0	X ¹ Σ _g ⁺	0	46.2	3.7906	4.0643
		1	138.2	3.6996	4.1752
		2	229.4	3.6394	4.2554
		3	319.9	3.5918	4.3230
		4	409.7	3.5516	4.3835
		5	498.8	3.5164	4.4391
		6	587.2	3.4848	4.4912
		7	674.9	3.4560	4.5407
		8	761.9	3.4294	4.5880
		9	848.1	3.4047	4.6337
		10	933.7	3.3815	4.6780
		11	1018.5	3.3597	4.7212
		12	1102.7	3.3389	4.7633
		13	1186.1	3.3192	4.8047
		14	1268.9	3.3003	4.8453
		15	1350.9	3.2822	4.8852
T _e = 15376.4 cm ⁻¹	B ¹ Π _u	0	37.4	4.0886	4.3929
		1	111.6	3.9885	4.5179
		2	185.1	3.9225	4.6089
		3	257.9	3.8706	4.6861
		4	330.0	3.8269	4.7553
		5	401.3	3.7886	4.8192
		6	472.0	3.7544	4.8794
		7	542.0	3.7233	4.9367
		8	611.2	3.6945	4.9917
		9	679.8	3.6678	5.0451
		10	747.6	3.6427	5.0970
		11	814.7	3.6190	5.1478
		12	881.0	3.5965	5.1978
		13	946.5	3.5749	5.2471
		14	1011.2	3.5542	5.2959
		15	1075.1	3.5341	5.3445

BIBLIOGRAPHY

- (08. 1) B \leftarrow X System,
R. W. Wood and T. S. Carter,
Phys. Rev. 27, 107-16
- (23. 2) A, B \leftarrow X Systems,
J. C. MacLennan and D. S. Ainslie,
Proc. Roy. Soc. A 103, 304-14
- (24. 3) B \leftarrow X System, Incorrect Analysis,
H. G. Smith,
Proc. Roy. Soc. A 106, 400-15
- (27. 4) B \leftarrow X System, Incorrect Analysis,
W. R. Fredrickson and W. W. Watson,
Phys. Rev. 30, 429-38
- (27. 5) B \leftarrow X System, Incorrect Analysis,
P. Pringsheim and B. Rosen,
Z. Physik 43, 519-23
- (28. 6) A, B \leftarrow X Systems,
R. Ritschl and D. Villars,
Naturwissenschaften 16, 219-20
- (28. 7) C \rightleftharpoons X System,
J. M. Walter and S. Barratt,
Proc. Roy. Soc. A 119, 257-75
- (29. 8) C \rightleftharpoons X System, Incorrect Constants,
H. Yamamoto,
Japan J. Phys. 5, 153-6
- (30. 9) C \rightleftharpoons X System,
W. Weizel and M. Kulp,
Ann. Phys. 4, 971-84
- (30. 10) A \leftarrow X System,
W. O. Crane and A. Christy,
Phys. Rev. 36, 421-9
- (30. 11) Theory,
E. Hutchinson,
Phys. Rev. 36, 410-20

- (31. 12) B \leftarrow X System, Rotational Analysis,
F. W. Loomis,
Phys. Rev. 38, 2153-61
- (31. 13) B \leftarrow X System,
F. W. Loomis and R. W. Wood,
Phys. Rev. 38, 854-6
- (32. 14) B \leftarrow X System,
F. W. Loomis,
Phys. Rev. 39, 189
- (32. 15) B \leftarrow X System, Vibrational Analysis, Dissociation Energy,
F. W. Loomis and R. E. Nusbaum,
Phys. Rev. 39, 89-98
- (32. 16) Band Polarization,
H. Kuhn,
Z. Physik 76, 782-92
- (36. 17) Band Polarization,
B. K. Chakraborti,
Indian J. Phys. 10, 155-62
- (37. 18) A \leftarrow X System,
T. Carroll,
Phys. Rev. 52, 822-35
- (37. 19) Ultraviolet Systems, Uncertain Analysis,
H. Yoshinaga,
Proc. Phys. -Math. Soc. Japan 19, 847-59
- (37. 20) Ultraviolet System, Uncertain Analysis,
H. Yoshinaga,
Proc. Phys. -Math. Soc. Japan 19, 1073-83
- (37. 21) Theory,
C. H. D. Clark,
Trans. Faraday Soc. 33, 1398-401
- (37. 22) Theory,
C. H. D. Clark and C. W. Scaife,
Trans. Faraday Soc. 33, 1394-8
- (39. 23) B \leftarrow X System,
W. W. Watson and W. F. Meggers,
J. Res. Nat. Bur. Stand. 20, 125-8

- (40.24) Theory,
G. B. B. M. Sutherland,
J. Chem. Phys. 8, 161-4
- (40.25) Theory,
R. F. Barrow,
Trans. Faraday Soc. 36, 624-5
- (40.26) Theory,
C. H. D. Clark,
Trans. Faraday Soc. 36, 370-6
- (41.27) Theory,
H. M. Hulburt and J. O. Hirschfelder,
J. Chem. Phys. 9, 61-9
- (47.28) Preliminary Note to (48.29),
R. W. B. Pearse and S. P. Sinha,
Nature 160, 159
- (48.29) C, D \rightleftharpoons X Systems,
S. P. Sinha,
Proc. Phys. Soc. 60, 436-43
- (49.30) S. P. Sinha,
Indian J. Phys. 23, 229-36
- (50.31) C \leftarrow X System, Vibrational Analysis,
S. P. Sinha,
Proc. Phys. Soc. A 63, 952-6
- (61.32) C \leftarrow X System, Rotational Analysis,
E. W. Robertson and R. F. Barrow,
Proc. Chem. Soc. 329-30
- (64.33) RKR Potential Energy Curves for B and X States,
D. K. Rai and A. N. Tripathi,
Can. J. Chem. 42, 452-7
- (64.34) Nuclear Magnetic Moment,
R. A. Brooks, C. H. Anderson, and N. F. Ramsey,
Phys. Rev. A 132, 62-8
- (66.35) Absorption Cross-Sections,
M. Lapp and L. P. Harris,
"Absorption Cross Sections of Alkali-Vapor Molecules: I. Cs₂ in the Visible, II. K₂ in the Red,"
J. Quant. Spectrosc. Radiative Transfer 6, 169-79

- (67. 36) Nonlinear Absorption of Ruby Laser Light,
V. G. Abramov, O. V. Konstantinov, N. N. Kostin, and V. A. Khadovoi,
"Nonlinear Absorption of Ruby Laser Light by Molecular Potassium
Vapor,"
Zh. Exsp. Teor. Fiz. 53, 822-30
- (68. 37) Absorption Cross-Sections,
D. M. Creek and G. V. Marr,
"Some Ultraviolet Cross-Section Measurements on Molecular Alkali-
Metal Vapours,"
J. Quant. Spectrosc. Radiative Transfer 8, 1431-6
- (68. 38) Theory,
L. Szasz and G. McGinn,
"Atomic and Molecular Calculations With the Pseudopotential Method.
III. The Theory of Li₂, Na₂, K₂, LiH, NaH, and KH,"
J. Chem. Phys. 48, 2997-3008
- (68. 39) B ← X System, Spectroscopic Analysis,
W. J. Tango, J. K. Link, and R. N. Zare,
"Spectroscopy of K₂ Using Laser-Induced Fluorescence,"
J. Chem. Phys. 49, 4264-8
- (69. 40) Potential Curves B, X States, RKR Potential,
D. C. Jain and R. C. Sahni,
"Reduced Potential Energy Curves of Some Electronic States of
Alkali Molecules,"
Trans. Faraday Soc. 65, 897-903
- (70. 41) Radiative Lifetime B State,
W. J. Tango and R. N. Zare, ¹Π_u State of K₂, "
J. Chem. Phys. 53, 3094-100
- (70. 42) Reaction With Cl,
W. S. Struve, T. Kitagawa, and D. R. Herschbach,
"Chemiluminescence in Molecular Beams: Electronic Excitation in
Reactions of Cl Atoms With Na₂ and K₂ Molecules,"
J. Chem. Phys. 54, 2759-61
- (70. 43) Potential Curves,
A. C. Roach and P. Baybutt,
"Potential Curves of Alkali Diatomic Molecules and the Origins of
Bonding Anomalies,"
Chem. Phys. Letters 7, 7-10

- (70. 44) Radiative Lifetime B State,
G. Baumgartner, W. Demtroder, and M. Stock,
"Lifetime-Measurements of Alkali-Molecules Excited by Different
Laserlines,"
Z. Physik 232, 462-72
- (71. 45) Production in Supersonic Expansion,
R. J. Gordon, Y. T. Lee, and D. R. Herschbach,
"Supersonic Molecular Beams of Alkali Dimers,"
J. Chem. Phys. 54, 2393-409
- (71. 46) Reactions With H and D Atoms,
Y. T. Lee, R. J. Gordon, and D. R. Herschbach,
"Molecular Beam Kinetics: Reactions of H and D Atoms with Diatomic
Alkali Molecules,"
J. Chem. Phys. 54, 2410-23
- (71. 47) Spectra From Heat Pipes,
P. P. Sorokin and J. R. Lankard,
"Emission Spectra of Alkali-Metal Molecules Observed With a Heat-
Pipe Discharge Tube,"
J. Chem. Phys. 55, 3810-3
- (71. 48) Optical Pumping,
G. Alzetta, A. Gozzini, and L. Moi,
"Effect of Atomic Orientation by Optical Pumping on the Formation of
the K₂ Molecule,"
C.R. Acad. Sci. B 274, 39-42
- (72. 49) Theory,
A. C. Roach,
"Theoretical Ground State and Excited State Potential Energy Curves
for Alkali Diatomic Molecules,"
J. Molec. Spectrosc. 42, 27-37
- (74. 50) Reactions With Halogens,
R. C. Oldenborg, J. L. Gole, and R. N. Zare,
"Chemiluminescent Spectra of Alkali-Halogen Reactions,"
J. Chem. Phys. 60, 4032-42
- (74. 51) R. W. Molof, T. M. Miller, H. L. Schwartz, B. Pederson, and J. T. Park,
"Measurements of the Average Electric Dipole Polarizabilities of the
Alkali Dimers,"
J. Chem. Phys. 61, 1816-22

Methods of Production and Experimental TechniqueAbsorption.

Emission: positive columns, condensed discharge, microwave discharge, electron beam discharge, α -particle irradiation.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$1,3\Sigma_u^- - 1\Sigma_g^+$	α irradiation	1250-1850		Max. $\sim 1480\text{\AA}$, 1280 \AA	Continuum	(73.9, 65.4, 55.3, 55.2)
	II	$B(1_u^-) - X^1\Sigma_g^+(0_g^+)$	Absorption	1252-1257	V	1254.8(3, 4)		(73.10)
	III	$C(0_u^+) - X^1\Sigma_g^+(0_g^+)$	Absorption	1239-1245		1241.3(3, 4) 1242.3(4, 4)		(73.10)
	IV	$D(0_u^+) - X^1\Sigma_g^+(0_g^+)$	Absorption	1167-1169		1168.1(2, 0) 1167.6(4, 1)		(73.10)
	V	$E - X^1\Sigma_g^+$	Absorption	1161-1170				(73.10)
	VI		Emission	2000-8000			Continuum	(67.7, 42.1)
	VII			1064-1080			4 fragmented systems	(73.10)
<p>Systems II - V correlate to separated atom limits in which one atom is excited to various levels of configuration $4p^55s$.</p> <p>System VII systems are energetically close to various atom levels of configuration $4p^55p$.</p>								

Molecule Kr₂

Kr₂

II. B(¹_u) ← X¹Σ_g⁺(⁰_g) System

Band heads, λ (Intensity) (73.10):

v', v''	0	1	2	3	4
0					1252.3(2)
1				1252.8(2)	1253.1(6)
2				1253.7(6)	1253.9(8)
3		1254.0(1)		1254.6(8)	1254.8(10)
4		1255.0(0)		1255.6(1)	1255.8(3)

III. C(⁰_u⁺) ← X¹Σ_g⁺(⁰_g) System

Band heads, λ (Intensity) (73.10):

v', v''	0	1	2	3	4
0				1239.2(9)	1239.5(9)
1		1239.2(9)	1239.5(7)	1239.8(8)	1240.0(10)
2	1239.6(6)	1239.9(7)	1240.2(8)	1240.4(8)	1240.7(9)
3	1240.2(4)	1240.6(4)	1240.9(5)	1241.1(6)	1241.3(10)
4	1241.0(1)	1241.4(3)	1241.6(5)	1241.9(8)	1242.1(10)

IV. D(⁰_u⁺) ← X¹Σ_g⁺(⁰_g) System

Band heads, λ (Intensity) (73.10):

v', v''	0	1	2	3	4
0	1169.2(5)	1169.5(4)	1169.7(3)	1170.0(2)	1170.1(1)
1	1168.6(8)	1168.9(5)	1169.2(5)	1169.4(2)	1169.6(2)
2	1168.1(8)	1168.4(2)	1168.7(3)	1168.9(5)	1169.1(3)
3	1167.7(6)	1168.0(7)	1168.2(2)	1168.4(2)	1168.7(3)
4	1167.3(7)	1167.6(8)	1167.8(5)		1168.2(2)

V. E ← X¹Σ_g⁺ System

Band heads in absorption, λ (Intensity) (73.10):

λ	1161.4	1162.3	1163.1	1163.7	1164.1	1164.4
(Intensity)	10	9	8	7	6	6

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e \omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$D(0_u^+)$	85531.5	(a) 39.66 (b)							(73.10)
$C(0_u^+)$	80763.9	(a) 35.75 (b)							(73.10)
$B(1_u)$	79932.8	22.3 (b)							(73.10)
$X^1\Sigma_g^+$ (0_g^+)	0	23.99	1.3	0.024	1.0			$y_e \omega_e = 0.021$	(73.11, 73.10)
(a) T_o ; (b) $\Delta G_{1/2}$ Dissociation energy = 0.02 eV, 0.39 kcal/mole, 138.4 cm^{-1} (73.10).									

Kr₂

Perturbations and General Information

Laser action has been observed on the $1,3\Sigma_u^+ \rightarrow X^1\Sigma_g^+$ transition at $1457 \pm 8\text{\AA}$ (73.13).

BIBLIOGRAPHY

- (42. 1) Observation,
B. Vogel,
Ann. Physik 41, 196-210
- (55. 2) Continuum in Condensed Discharge,
Y. Tanaka,
J. Opt. Soc. Am. 45, 710-3
- (55. 3) Observation in Microwave Discharge,
P. G. Wilkinson,
J. Opt. Soc. Am. 45, 1044-6
- (65. 4) Observation in Microwave Discharge,
P. G. Wilkinson and E. T. Byram,
Appl. Opt. 4, 581-8
- (65. 5) Observation of Continuum,
R. E. Huffman, J. C. Larrabee, and Y. Tanaka,
Appl. Opt. 4, 1581-8
- (66. 6) Ionization Potential,
J. A. R. Samson and R. B. Cairns,
J. Opt. Soc. Am. 56, 769-75
- (67. 7) Formation of Molecule,
J. F. Prince and W. W. Robertson,
J. Chem. Phys. 46, 3309-13
- (68. 8) R. Turner and H. D. Riccius,
"Visible Afterglow Emission of Krypton,"
J. Chem. Phys. 48, 4351-6
- (73. 9) $1,3\Sigma_g^+ \rightarrow X^1\Sigma_g^+$ Emission,
A. Gedanken, B. Raz, and J. Jortner,
"Emission Spectra of Homonuclear Diatomic Rare Gas Molecules in
Solid Neon,"
J. Chem. Phys. 59, 1630-3
- (73. 10) Absorption,
Y. Tanaka, K. Yoshino, and D. E. Freeman,
"Vacuum Ultraviolet Absorption Spectra of the Van Der Waals
Molecules Kr₂ and ArKr,"
J. Chem. Phys. 59, 5160-83

- (73. 11) Ground State Potential,
K. K. Docken and T. P. Schafer,
"Spectroscopic Information in Ground-State Ar₂, Kr₂, and Xe₂ From
Interatomic Potentials,"
J. Molec. Spectrosc. 46, 454-9

- (73. 12) Interatomic Potential,
U. Buck, M. G. Dondi, U. Valbusa, M. L. Klein, and G. Scoles,
"Determination of the Interatomic Potential of Krypton,"
Phys. Rev. A 8, 2409-16

- (73. 13) P. W. Hoff, J. C. Swingle, and C. K. Rhodes,
"Observations of Stimulated Emission From High Pressure Krypton
and Argon/Xenon Mixtures,"
Appl. Phys. Letters 23, 245-8

- (74. 14) D. W. Gough, E. B. Smith, and G. C. Maitland,
"The Pair Potential Energy Function for Krypton,"
Molec. Phys. 27, 867-72

La₂Methods of Production and Experimental Technique

Thermal emission from a King furnace ($T > 2000^{\circ}\text{C}$).

Band Systems

Bands in the region 6100-6040Å have been attributed to La₂. The bands are degraded principally to the violet, but the series convergence is degraded red (69.2).

Characteristic bands:

λ | 6075.3 | 6074.9 | 6074.7 | 6074.6 | 6069.4 | 6068.8 | 6049.6 | 6049.1

A vibrational analysis yields $\omega'_0 = 82.6 \text{ cm}^{-1}$ and $\omega''_0 = 76.9 \text{ cm}^{-1}$, but these values are in doubt.

Spectroscopic Constants

Dissociation energy = $2.50 \pm 0.22 \text{ eV}$, 57.6 kcal/mole , 20200 cm^{-1} (64.1).

BIBLIOGRAPHY

- (64. 1) Dissociation Energy,
G. Verhaegen, S. Smoes, and J. Drowart,
J. Chem. Phys. 40, 239-41
- (69. 2) Emission, Vibrational Analysis,
P. Carette and J.M. Blondeau,
C.R. Acad. Sci. 269, 16-18

Methods of Production and Experimental Technique

Absorption, magnetic rotation.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$A^1\Sigma_u^+ - X^1\Sigma_g^+$	Absorption	7700-6550	R	6883.9(2, 0)		(72.64, 29.16, 28.1)
	II	$B^1\Pi_u - X^1\Sigma_g^+$	Absorption	5590-4500	R	4800.6(3, 1) 4778.8(2, 0)		(33.13, 31.9)
	III	$C^1\Pi_u - X^1\Sigma_g^+$	Absorption	3500-3100	R	3358.6(0, 2) 3315.6(0, 1)		(60.36, 38.31)
	IV	$D^1\Pi_u - X^1\Sigma_g^+$	Absorption	3100-2500	R			(60.36)
Several bands of the isotopic species $^7\text{Li}^6\text{Li}$ have been observed for Systems II and III.								

Molecule Li₂

Li₂

I. A¹Σ_u⁺ ← X¹Σ_g⁺ System

Most intense band heads, λ (Intensity) (36.16, 28.1):

(v', v'')	(0, 2)	(0, 1)	(1, 1)	(1, 0)	(2, 0)	(3, 0)
λ	7690.3	7309.2	7177.4	7003.7	6883.9	6768.7
(Intensity)	8	8	8	8	10	8

II. B¹Π_u ← X¹Σ_g⁺ System

Most intense band heads of ⁷Li₂, λ (Intensity) (31.9):

(v', v'')	(2, 1)	(1, 0)	(3, 1)	(2, 0)	(4, 1)	(3, 0)
λ	4859.7	4838.2	4800.6	4778.8	4744.9	4722.0
(Intensity)	1.5	4	10	10	4	1.5

Most intense band heads of ⁷Li⁶Li, λ (Intensity) (31.9):

(v', v'')	(0, 0)	(1, 0)	(4, 1)
λ	4901.8	4836.5	4739.7
(Intensity)	5	4	2

III. C¹Π_u ← X¹Σ_g⁺ System

Most intense band heads, λ (Intensity) (60.36, 48.31):

(v', v'')	(0, 4)	(1, 4)	(0, 3)	(2, 4)	(0, 2)	(0, 1)	(0, 0)	(1, 0)
λ	3431.2	3404.4	3392.1	3378.5	3358.6	3315.6	3277.6	3253.1
(Intensity)	4	4	6	4	10	9	6	10

IV. D¹Π_u ← X¹Σ_g⁺ System

Several systems are superimposed in the region 3100-2500Å. Simple Q branches here have been attributed to a D¹Π_u ← X¹Σ_g⁺ system. The D state appears perturbed (60.36).

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e \omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$D^1\Pi_u$	≤ 34140	~ 205		0.465			3.18		(60.36)
$C^1\Pi_u$	30549	237.9	3.33	0.5068	9.39	9.9	3.08	$y_e \omega_e = 0.060$	(60.36)
$B^1\Pi_u$	20439.40	270.94	3.13	0.5577	8.88	9.45	2.93	$y_e \omega_e = -0.0637$	(33.13, 3.9)
$A^1\Sigma_u^+$	14069.9	255.50	1.59	0.4975	5.22		3.11	$y_e \omega_e = 0.0039$ (a)	(36.16, 28.1)
$X^1\Sigma_g^+$	0	351.43	2.55	0.672	6.8	9.87	2.67	(b)	(69.51, 36.16, 28.1)
(a) Spectroscopic constants for $^6\text{Li}_2$ (72.64); (b) spectroscopic constants for $^6\text{Li}_2$, $^7\text{Li}^6\text{Li}$ (69.31) Dissociation energy = 1.026 ± 0.006 eV, 23.66 kcal/mole, 8275 cm^{-1} (69.51).									

Li₂

Perturbations and General Information

Gyromagnetic ratio (g_j) = 0.10797 nuclear magnetons (64.39).

Transition probabilities (70.53):

Transition	ν	f
$A^1\Sigma_u^+ - X^1\Sigma_u^+$	14068	0.8688
$C^1\Pi_u - X^1\Sigma_u^+$	30558	0.0158

Average polarizability (990°K) = $34 \times 10^{-24} \text{ cm}^3$ (74.68).

Potential energy curves - RKR potentials (69.50):

	State	ν	$U(\text{cm}^{-1})$	$r_{\min}(\text{\AA})$	$r_{\max}(\text{\AA})$
$T_e = 0.0$	$X^1\Sigma_g^+$	0	175.1	2.5163	2.8480
		1	521.3	2.4131	2.9911
		2	862.3	2.3470	3.0980
		3	1198.0	2.2961	3.1906
		4	1528.4	2.2542	3.2752
		5	1853.5	2.2183	3.3548
		6	2173.2	2.1868	3.4309
		7	2487.5	2.1588	3.5046
		8	2796.4	2.1336	3.5766
		9	3099.7	2.1107	3.6475
		10	3397.6	2.0897	3.7175
		11	3689.9	2.0704	3.7872
		12	3976.6	2.0526	3.8566
		13	4257.7	2.0361	3.9260
		14	4533.2	2.0203	3.9956
		15	4802.9	2.0066	4.0656
		16	5067.0	1.9935	4.1361
$T_e = 14069.9 \text{ cm}^{-1}$	$A^1\Sigma_u^+$	0	127.3	2.9237	3.3125
		1	379.7	2.8043	3.4812
		2	628.8	2.7281	3.6066
		3	874.9	2.6693	3.7142
		4	1117.9	2.6205	3.8116
		5	1357.7	2.5782	3.9021

$T_e = 20439.40 \text{ cm}^{-1}$	State	v	$U(\text{cm}^{-1})$	$r_{\min}(\text{\AA})$	$r_{\max}(\text{\AA})$
	$B^1\Pi_u$				
		0	134.2	2.7598	3.1389
		1	398.2	2.6448	3.3074
		2	656.1	2.5714	3.4354
		3	907.6	2.5148	3.5480
		4	1152.2	2.4675	3.6526
		5	1389.7	2.4263	3.7528
		6	1619.6	2.3893	3.8506
		7	1841.5	2.3552	3.9476
		8	2055.0	2.3232	4.0449
		9	2259.8	2.2927	4.1434
		10	2455.5	2.2631	4.2441
		11	2641.7	2.2339	4.3479
		12	2814.6	2.2016	4.4635
		13	2976.8	2.1704	4.5812
		14	3127.9	2.1384	4.7059

BIBLIOGRAPHY

- (28. 1) A \leftarrow X System, Vibrational Analysis,
K. Wurm,
Naturwissenschaften 16, 1028
- (29. 2) B \leftarrow X System, Rotational Analysis,
A. Harvey and F. A. Jenkins,
Phys. Rev. 34, 1286
- (29. 3) B \leftarrow X System, Rotational Analysis,
K. Wurm,
Z. Physik 58, 562-9
- (29. 4) A \leftarrow X System, Rotational Analysis,
K. Wurm,
Z. Physik 59, 35-41
- (30. 5) B \leftarrow X System, Rotational Analysis,
A. Harvey and F. A. Jenkins,
Phys. Rev. 35, 132
- (30. 6) B \leftarrow X System, Rotational Analysis,
A. Harvey and F. A. Jenkins,
Phys. Rev. 35, 789-801
- (31. 7) Comparison With Theory,
J. H. Bartlett and W. H. Furry,
Phys. Rev. 37, 1712
- (31. 8) B \leftarrow X System, Rotational Analysis,
F. W. Loomis and R. E. Nusbaum,
Phys. Rev. 37, 1712
- (31. 9) B \leftarrow X System, Vibrational Analysis, Dissociation Energy,
F. W. Loomis and R. E. Nusbaum,
Phys. Rev. 38, 1447-57
- (31. 10) Theory,
W. R. Van Wijk and A. J. Van Koeveeringe,
Proc. Roy. Soc. A 132, 98-107
- (33. 11) Theory,
W. H. Furry,
Phys. Rev. 43, 361-2

- (33. 12) Comparison Between $^6\text{Li}_2$ and $^7\text{Li}_2$,
F. A. Jenkins and A. MacKellar,
Phys. Rev. 44, 325-6
- (33. 13) B \leftarrow X System, Rotational Analysis,
A. MacKellar,
Phys. Rev. 44, 155-64
- (35. 14) Preliminary Note to (36.16),
G. M. Almy and G. R. Irwin,
Phys. Rev. 48, 104-5
- (35. 15) C \leftarrow X System, Ultraviolet Systems,
J. E. Vance and J. R. Huffman,
Phys. Rev. 47, 215-6
- (36. 16) A \leftarrow X System, Rotational Analysis,
G. M. Almy and G. R. Irwin,
Phys. Rev. 49, 72-7
- (37. 17) Theory,
H. Yoshinaga,
Proc. Phys. -Math. Soc. Japan 19, 847-59
- (37. 18) Theory,
H. Yoshinaga,
Proc. Phys. -Math. Soc. Japan 19, 1073-83
- (39. 19) Theory,
C. H. D. Clark,
Nature 144, 285-6
- (40. 20) Theory,
M. F. Mamotenko,
Acta Physicochim. 12, 946-7
- (40. 21) Theory,
G. B. B. M. Sutherland,
J. Chem. Phys. 8, 161-4
- (40. 22) Theory,
R. F. Barrow,
Trans. Faraday Soc. 36, 624-5
- (40. 23) Theory,
C. H. D. Clark,
Trans. Faraday Soc. 36, 370-6

- (40.24) Theory,
J. W. Linnett,
Trans. Faraday Soc. 36, 1123-34
- (41.25) Theory,
H. M. Hulburt and J. O. Hirschfelder,
J. Chem. Phys. 9, 61-9
- (41.26) Theory,
C. H. D. Clark,
Trans. Faraday Soc. 37, 299-302
- (41.27) Theory,
C. H. D. Clark and K. R. Welb,
Trans. Faraday Soc. 37, 293-8
- (42.28) Theory,
H. Fajans,
J. Chem. Phys. 10, 759-60
- (42.29) Theory,
K. Fajans,
J. Chem. Phys. 10, 761
- (47.30) Preliminary Note to (48.31),
R. W. B. Pearse and S. P. Sinha,
Nature 160, 159
- (48.31) C ← X System,
S. P. Sinha,
Proc. Phys. Soc. 60, 443-7
- (53.32) Calculation of Magnetic Properties,
R. M. Sternheimer and H. M. Foley,
Phys. Rev. 92, 1460-8
- (57.33) Theory,
R. Fieschi,
Ist. Naz. Fiz. Nucl. Milano 112, 195
- (57.34) Theory,
E. Ishiguro, K. Kayama, M. Kotani, and Y. Mizuno,
J. Phys. Soc. Japan 12, 1355-85
- (58.35) Theory,
T. Arai and M. Sakamoto,
J. Chem. Phys. 28, 32-48

- (60. 36) C, D X Systems,
R. F. Barrow, N. Travis, and C. V. Wright,
Nature 187, 141-2
- (60. 37) LCAO-MO-SCF Calculations,
B. J. Ransil,
Rev. Mod. Phys. 32, 400-11
- (63. 38) VB Calculations,
C. Manneback,
Physica 29, 769-83
- (64. 39) Rotational Magnetic Moment,
R. A. Brooks, C. H. Anderson, and N. F. Ramsey,
Phys. Rev. 136, 62-8
- (65. 40) Magnetic Properties,
R. M. Stevens and W. N. Lipscomb,
J. Chem. Phys. 42, 4302-4
- (66. 41) LCAO-MO-SCF Calculations,
G. Das and A. C. Wahl,
J. Chem. Phys. 44, 87-96
- (67. 42) Extended Hartree-Fock Calculations,
G. Das,
J. Chem. Phys. 46, 1568-78
- (67. 43) Calculated Molecular Properties,
W. D. Lyon and J. O. Hirschfelder,
J. Chem. Phys. 46, 1788-96
- (67. 44) AMO Calculations,
D. K. Rai and J. L. Calais,
J. Chem. Phys. 47, 906-11
- (67. 45) J. R. De La Vega and H. F. Hameka,
"Calculation of Magnetic Susceptibilities of Diatomic Molecules. V.
Homomuclear Molecules,"
Physica 35, 313-22
- (67. 46) J. R. De La Vega and H. F. Hameka,
"Calculation of Magnetic Susceptibilities of Diatomic Molecules. VIII.
Anisotropies and Rotational Magnetic Moments,"
J. Chem. Phys. 47, 1834-6

- (68. 47) M. A. Marchetti and S. R. LaPaglia,
"Theoretical $1\Sigma_g^+$ - $1\Sigma_u^+$ Dipole Strengths of Some Homonuclear Diatomic Molecules: Configuration Interaction,"
J. Chem. Phys. 48, 434-9
- (68. 48) L. Szasz and G. McGinn,
"Atomic and Molecular Calculations With the Pseudopotential Method. III. The Theory of Li₂, Na₂, K₂, LiH, NaH, and KH,"
J. Chem. Phys. 48, 2997-3008
- (69. 49) P. Colmant and Ch. Manneback,
"Electronic Structure and Energy of the Homonuclear Molecule Li₂ in its $1\Sigma_g^+$ Ground State,"
Bull. Cl. Sci. Acad. Rol. Belg. 55, 55-84
- (69. 50) D. C. Jain and R. C. Sahni,
"Reduced Potential Energy Curves of Some Electronic States of Alkali Molecules,"
Trans. Faraday Soc. 65, 897-903
- (69. 51) R. Velasco, Ch. Ottinger, and R. N. Zare,
"Dissociation Energy of Li₂ From Laser-Excited Fluorescence,"
J. Chem. Phys. 51, 5522-32
- (70. 52) W. Kutzelnigg and M. Gelus,
"Potential Curve of the Li₂ Ground State for Large Internuclear Distances. A Contribution to the Understanding of Interatomic Forces,"
Chem. Phys. Letters 7, 296-302
- (70. 53) A. N. Singh and D. K. Rai,
"Transition Probabilities for Electronic Spectra of Li₂ and C₂,"
Proc. Nat. Acad. Sci. A 40, 101-2
- (70. 54) J. N. Bardsley,
"Pseudopotential Calculations of Alkali Interactions,"
Chem. Phys. Letters 7, 517
- (71. 55) A. K. Chandra and R. Sundar,
"A View of Bond Formation in the Li₂ Molecule,"
Molec. Phys. 22, 369-74
- (71. 56) Ch. Ottinger and D. Poppe,
"Collision-Induced Rotational and Vibrational Quantum Jumps in Electronically Excited Li₂,"
Chem. Phys. Letters 8, 513-8

- (72. 57) W. von Niessen,
"Density Localization of Atomic and Molecular Orbitals. II. Homonuclear Diatomic Molecules,"
Theoret. Chim. Acta 27, 9-23
- (72. 58) G. L. Bendazzoli, F. Bernardi, and A. Geremia,
"A. M. O. Calculations for Some First Row Diatomic Molecules,"
Theoret. Chim. Acta 27, 63-8
- (72. 59) W. Kutzelnigg, V. Staemmler, and M. Gelus,
"Potential Curve of the Lowest Triplet State of Li₂,"
Chem. Phys. Letters 13, 496-500
- (72. 60) S. Kohda, K. Ohno, and H. Taketa,
"On the First Singlet and Triplet Excited States of the Lithium Molecule,"
Bull. Chem. Soc. Japan 45, 2737-8
- (72. 61) G. C. Shukla,
"An Improved AMO Function for the Li₂ Molecule,"
Acta Phys. Polon. A41, 683-7
- (72. 62) A. C. Roach,
"Theoretical Ground State and Excited State Potential Energy Curves for Alkali Diatomic Molecules,"
J. Molec. Spectrosc. 42, 27-37
- (72. 63) A. Hernandez and E. V. Ludena,
"Loge Localization Analysis of Diatomic Molecules: Li₂ and F₂,"
J. Chem. Phys. 57, 5350-3
- (72. 64) R. Velasco and F. Rivero,
"The A - X Bands System of the ⁶Li₂ Molecule,"
Opt. Pura Appl. 5, 76-9
- (73. 65) T. Caves,
"Van Der Waals Interactions Between Excited Li Atoms,"
J. Chem. Phys. 59, 6177-82
- (73. 66) R. Velasco and V. Morales,
"The B - X Band System of the ⁶Li₂ Molecule,"
Opt. Pura Appl. 6, 52-6
- (74. 67) G. C. Lie and E. Clementi,
"Study of the Electronic Structure of Molecules. XXII. Correlation Energy Corrections as a Function of the Hartree-Fock Type Density and its Application to the Homonuclear Diatomic Molecules of the Second Row Atoms,"
J. Chem. Phys. 60, 1288-96

Li₂

- (74. 68) R. W. Molof, T. M. Miller, H. L. Schwartz, B. Bederson, and J. T. Park,
"Measurements of the Average Electric Dipole Polarizabilities of the Alkali Dimers,"
J. Chem. Phys. 61, 1816-22
- (74. 69) G. Ennen and Ch. Ottinger,
"Rotation - Vibration - Translation Energy Transfer in Laser Excited Li₂ ($B^1 \Pi_u$),"
Chem. Phys. 3, 404-30

Methods of Production and Experimental Technique

Absorption (T ~ 800° C).

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$A^1\Sigma_u^+ - X^1\Sigma_g^+$	Absorption	3853-3140	V	3790. 9(0, 2) 3764. 7(0, 3)		(70.7)
	II	$(^1\Pi_u) - X^1\Sigma_g^+$	Absorption	2852-2660	-			(70.7)

Molecule
Mg₂

Mg₂

I. A¹Σ_u⁺ ← X¹Σ_g⁺ System

Band heads, λ (70.7):

v', v''	3	4	5	6	7
2	3790.9	3796.5	3801.6	3806.3	3810.7
3	3764.6	3770.2	3775.3	3779.9	3784.2
4	3739.2	3744.5	3749.5	3754.2	3758.3
5	3714.2	3719.5	3724.5	3729.0	

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$\times_e \omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$A^1\Sigma_u^+$	26068.76	190.615	1.14562	0.147999	1.31642	0.334286	3.082		(70.7)
$X^1\Sigma_g^+$	0	51.12	1.6448	0.0929	3.7758	1.2166	3.890		(70.7)
Dissociation energy = 0.05 eV, 1.15 kcal/mole, 404.1 cm^{-1} (73.10).									

Mg₂

Perturbations and General Information

Potential energy curves - RKR potentials (72.8):

	State	v	E(v)cm ⁻¹	r _{min} (Å)	r _{max} (Å)
T _e = 0.0	X ¹ Σ _g ⁺	0	25.156	3.6872	4.1626
		1	73.037	3.5698	4.4165
		2	117.757	3.5010	4.6260
		3	159.384	3.4509	4.8226
		4	197.971	3.4112	5.0166
		5	233.558	3.3786	5.2140
		6	266.168	3.3513	5.4195
		7	295.811	3.3285	5.6380
		8	322.482	4.4097	5.8750
		9	346.162	3.2948	6.1378
		10	366.806	3.2835	6.4364
		11	384.393	3.2762	6.7852
		12	398.831	3.2717	7.2110
T _e = 26068.76 cm ⁻¹	A ¹ Σ _u ⁺	0	95.021	2.9676	3.2111
		1	283.350	2.8915	3.3154
		2	469.404	2.8426	3.3927
		3	653.193	2.8048	3.4591
		4	834.728	2.7736	3.5193
		5	1014.020	2.7467	3.5754
		6	1191.078	2.7231	3.6286
		7	1365.915	2.7018	3.6796
		8	1538.541	2.6826	3.7290
		9	1708.965	2.6649	3.7771
		10	1877.199	2.6486	3.8242
		11	2043.254	2.6335	3.8704
		12	2207.139	2.6193	3.9150
		13	2368.867	2.6060	3.9609
		14	2528.446	2.5935	4.0055
		15	2685.889	2.5818	4.0497

Franck-Condon factors - RKR potentials (72.8):

$A^1\Sigma_u^+ - X^1\Sigma_g^+$

v', v''	0	1	2	3	4	5	6	7	8
0	0.0000	0.0000	0.0001	0.0003	0.0006	0.0010	0.0014	0.0019	0.0022
1	0.0001	0.0004	0.0012	0.0027	0.0047	0.0070	0.0092	0.0110	0.0121
2	0.0004	0.0020	0.0053	0.0102	0.0159	0.0211	0.0249	0.0266	0.0264
3	0.0016	0.0065	0.0148	0.0245	0.0326	0.0370	0.0371	0.0337	0.0283
4	0.0044	0.0157	0.0301	0.0412	0.0448	0.0406	0.0316	0.0216	0.0130
5	0.0103	0.0302	0.0471	0.0508	0.0416	0.0264	0.0126	0.0039	0.0004
6	0.0204	0.0480	0.0578	0.0452	0.0235	0.0067	0.0002	0.0014	0.0055
7	0.0350	0.0636	0.0550	0.0259	0.0045	0.0004	0.0067	0.0138	0.0169
8	0.0530	0.0707	0.0381	0.0061	0.0011	0.0121	0.0210	0.0212	0.0156
9	0.0722	0.0653	0.0160	0.0004	0.0147	0.0261	0.0228	0.0124	0.0039
10	0.0895	0.0485	0.0015	0.0120	0.0297	0.0248	0.0099	0.0009	0.0008

BIBLIOGRAPHY

- (31. 1) H. Hamada,
Nature 127, 555
- (31. 2) H. Hamada,
Philos. Mag. 12, 50-67
- (55. 3) Dissociation Energy,
J. R. Soulen, P. Sthapitanonda, and J. L. Margrave,
J. Phys. Chem. 59, 132-6
- (64. 4) S. Weniger,
J. Phys. 25, 946-9
- (70. 5) R. H. Ewing and A. M. Mellor,
"Further Calculations of Equilibrium Dimer Properties,"
J. Chem. Phys. 53, 2983-4
- (70. 6) W. C. Stwalley,
"Long-Range Analysis of the Internuclear Potential of Mg₂,"
Chem. Phys. Letters 7, 600-2
- (70. 7) W. J. Balfour and A. E. Douglas,
"Absorption Spectrum of the Mg₂ Molecule,"
Can. J. Phys. 48, 901-14
- (72. 8) W. J. Balfour and R. F. Whitlock,
"Rotational Dependence of Franck-Condon Factors in the $A^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$
System of ²⁴Mg₂,"
Can. J. Phys. 50, 1648-51
- (72. 9) A. C. Brett and C. Chan,
"The Mg₂ Potential: A Curve Fitting Study,"
Can. J. Phys. 50, 1587-9
- (73. 10) K. C. Li and W. C. Stwalley,
"Vibrational Levels Near Dissociation in Mg₂ and Long Range Forces,"
J. Chem. Phys. 59, 4423-7
- (73. 11) M. K. Matzen, G. V. Calder, and D. K. Hoffman,
"An Accurate Semi-Empirical Potential Function for Diatomic
Molecules,"
Spectrochim. Acta 29A, 2005-16

Mn₂Spectroscopic Constants

Dissociation energy = 0.22 ± 0.17 eV, 5 kcal/mole, 1750 cm^{-1} (68.2).



BIBLIOGRAPHY

- (64. 1) A. Kant and B. Strauss,
"Dissociation Energies of Diatomic Molecules of the Transition
Elements. II. Titanium, Chromium, Manganese, and Cobalt,"
J. Chem. Phys. 4, 3806-8
- (68. 2) A. Kant, S. Lin, and B. Strauss,
"Dissociation Energy of Mn₂,"
J. Chem. Phys. 49, 1983-5

Methods of Production and Experimental Technique

Absorption (in the vacuum ultraviolet).

Emission from discharge into air, pure N₂, or N₂ in rare gases, hollow cathode discharge, high voltage arc, afterglow, aurora, laser emission, electron beam emission.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
Vegard- Kaplan Wilkinson Saum- Benesch Ogawa- Tanaka- Wilkinson	I	$A^3\Sigma_u^+ \leftarrow X^1\Sigma_g^+$	Luminescence	5060-2100	R	2760.8(0, 6)		(71.105, 68.80, 68.75, 65.57, 62.40, 61.38, 59.31, 34.6, 34.5, 32.3)
	II	$B^3\Pi_g \leftarrow X^1\Sigma_g^+$	Absorption	1690-1630	R	1635(0, 0) 1638(1, 0)		(62.42)
	III	$W^3\Delta_u \leftarrow X^1\Sigma_g^+$	Absorption	4400-2400				(71.101)
	IV	$B^1\Sigma_u^- \leftarrow X^1\Sigma_g^+$	Absorption	2240-1120	R			(65.51, 64.46)

Molecule N₂

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
Ogawa-Tanaka- Wilkinson-Mulliken Lyman-Birge- Hopfield Tanaka Tanaka	V	$a'^1\Sigma_u^- \rightarrow X'^1\Sigma_g^+$	Absorption: N ₂ + Ar	2000-1080	R			(66.62, 65.54, 64.46, 60.35, 59.32, 59.30)
	VI	$a'^1\Pi_g \rightarrow X'^1\Sigma_g^+$	Absorption and discharge	2600-1090	R	2125.0(5, 14) 2041.2(5, 13)		(66.63, 65.59, 65.55, 54.46, 56.25)
	VII	$w'^1\Delta_u \rightarrow X'^1\Sigma_g^+$	Absorption	1400-1140	R			(64.46)
	VIII	$C'^3\Pi_u \rightarrow X'^1\Sigma_g^+$	Absorption	1130-1070	R		5 heads	(65.53, 64.46)
	IX	$E'^3\Sigma_g^+ \rightarrow X'^1\Sigma_g^+$	Energy loss spectra	~ 1050		1043.9(0, 0)		(73.166)

Molecule N₂

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
Dressler- Lutz	X	$a'^1\Sigma_g^+ \rightarrow X'^1\Sigma_g^+$	Absorption	~ 1010		1011.5(0, 0)		(73.166, 67.67)
	XI	$b'^1\Pi_u \rightarrow X'^1\Sigma_g^+$	Absorption and discharge	995-855	R	979.5(2, 0)		(73.166, 69.83, 69.82, 69.81, 64.47)
	XII	$F'^3\Pi_u \rightarrow X'^1\Sigma_g^+$	Energy loss spectra	980-930		972.2(0, 0)		(73.166)
	XIII	$G'^3\Pi_u \rightarrow X'^1\Sigma_g^+$	Energy loss spectra	970-940		967.7(0, 0)		(73.166)
	XIV	$D'^3\Sigma_u^+ \rightarrow X'^1\Sigma_g^+$	Energy loss spectra	~ 960		965.4(0, 0)		(73.166)
	XV	$b'^1\Sigma_u^+ \rightarrow X'^1\Sigma_g^+$	Absorption and discharge	965-830	R			(69.83, 69.82, 69.81, 64.47)
	XVI	$c'^1\Pi_u \rightarrow X'^1\Sigma_g^+$	Absorption and discharge	960-865	R			(69.83, 69.82, 69.81, 64.47)
	XVII	$c'^1\Sigma_u^+ \rightarrow X'^1\Sigma_g^+$	Absorption and discharge	960-840	R			(69.83, 69.82, 69.81, 64.47)

Molecule N₂

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
First Positive Hermans-Kaplan-Wu-Benesch Bands	XVIII	$\text{o}^1\Pi_u \rightarrow \text{X}^1\Sigma_g^+$	Absorption and discharge	950-880	R			(69.83, 69.82, 69.81, 64.47)
	XIX	$\text{e}^1\Pi_u \rightarrow \text{X}^1\Sigma_g^+$	Energy loss spectra	~ 860		865.1(0, 0)		(69.90)
	XX	$\text{e}^1\Sigma_u^+ \rightarrow \text{X}^1\Sigma_g^+$	Energy loss spectra	~ 860		863.8(0, 0)		(69.90)
	XXI	$\text{B}^3\Pi_g \rightarrow \text{A}^3\Sigma_u^+$	Positive column	Infrared - 4700	V	10510.1(0, 0) 8912.4(1, 0)		(61.38, 59.33)
	XXII	$\text{E}^3\Sigma_g^+ \rightarrow \text{A}^3\Sigma_u^+$	Luminescence	2740-2130	V	2471.4(0, 4) 2391.1(0, 3)	Bands not resolved	(45.16, 35.9)
	XXIII	$\text{W}^3\Delta_u \rightarrow \text{B}^3\Pi_g$	Discharge	69000-7000			Bands not resolved	(71.101, 68.73)
	XXIV	$\text{B}^3\Sigma_u^- \rightarrow \text{B}^3\Pi_g$	Luminescence from discharge	8920-6060	R		Complex structure	(64.45, 60.36, 60.34, 58.29)

Molecule N₂

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
Secora Goldstein-Fourth Positive MacFarlane Bands	XXV	$\text{C}^3\Pi_u \rightarrow \text{B}^3\Pi_g$	Positive column	5450-2680	V	3371.3(0, 0) 3576.9(0, 1)		(65.56, 62.49, 60.37, 59.33)
	XXVI	$\text{C}^3\Pi_u \rightarrow \text{B}^3\Pi_g$	Luminescence	5060-2860	R	4728.0(0, 11)		(64.45, 63.44, 61.38)
	XXVII	$\text{D}^3\Sigma_u^+ \rightarrow \text{B}^3\Pi_g$	Luminescence from discharge	2910-2250	V	2448.0(0, 2)	5 heads	(40.11)
	XXVIII	$\text{E}^3\Sigma_g^+ \rightarrow \text{B}^3\Pi_g$	Electron impact	3180-2740	V	2740(0, 0)		(69.88)
	XXIX	$\text{a}^1\Pi_g \rightarrow \text{a}^1\Sigma_u^-$	Laser emission	82000-33000				(65.58)
	XXX	$\text{x}^1\Sigma_g^- \rightarrow \text{a}^1\Sigma_u^-$	Discharge	2850-2030	V	2411.7(1, 4)		(56.26)

Molecule N₂

N₂

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
First Kaplan MacFarlane Infrared Gaydon- Herman Gaydon- Herman Gaydon- Herman Gaydon- Herman	XXXI	$y^1\Pi_g \rightarrow a^1\Sigma_u^-$	Discharge	2470-2070	V	2225.9(0, 1)		(57.28)
	XXXII	$w^1\Delta_u \rightarrow a^1\Pi_g$	Laser emission	36500				(66.64)
	XXXIII	$b^1\Pi_u \rightarrow a^1\Pi_g$	Discharge	3420-2740	R			(69.82, 69.81, 57.27)
	XXXIV	$b^1\Sigma_u^+ \rightarrow a^1\Pi_g$	Discharge	2500	R			(69.82, 69.81, 57.27)
	XXXV	$c^1\Pi_u \rightarrow a^1\Pi_g$	Discharge	3010-2220	R, V			(69.82, 69.81, 57.27)
	XXXVI	$c^1\Sigma_u^+ \rightarrow a^1\Pi_g$	Discharge	3660-2280	R, V			(69.82, 69.81, 57.27)

Molecule N₂

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
Gaydon- Herman Gaydon- Herman Second Kaplan XL XLI Gaydon Green Herman Infrared	XXXVII	$d^1\Pi_u \rightarrow a^1\Pi_g$	Discharge	2550-2350				(69.82, 69.81, 57.27)
	XXXVIII	$b^1\Pi_u \rightarrow a^1\Pi_g$	Discharge	2860-2720	R			(69.82, 69.81, 57.27)
	XXXIX	$y^1\Pi_g \rightarrow w^1\Delta_u$	Discharge	2860-2260	V	2536.6(0, 2)		(57.28)
	XL	$z^1\Delta_g \rightarrow w^1\Delta_u$	Discharge	2480-2360	V			(57.27)
	XLI	$E^3\Sigma_g^+ \rightarrow C^3\Pi_u$	Electron impact	12850	V	12843.6(0, 0)	One band observed	(69.88)
	XLII	?	Discharge	6340-5040	V	5815(0, 1)	Bands not resolved	(54.23, 53.22, 44.15)
	XLIII	?	Discharge	8550-7000	V	8057(0, 0)		(53.22, 51.18)

Molecule N₂

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
Molecule N ₂	Worley-Jenkins XLIV	$X^2\Sigma_g^+ - X^1\Sigma_g^+$ (N ₂ ⁺)	Absorption	< 960			Rydberg series	(69.82, 69.81, 67.66, 62.39, 53.21, 53.20, 43.14, 42.13)
	Carroll-Yoshino XLV	$X^2\Sigma_g^+ - X^1\Sigma_g^+$ (N ₂ ⁺)	Absorption				Rydberg series	(69.82, 69.81, 67.66)
	Worley XLVI	$A^2\Pi_u - X^1\Sigma_g^+$ (N ₂ ⁺)	Absorption	< 960			Rydberg series	(62.39, 53.21, 53.20)
	Hopfield XLVII	$B^3\Sigma_u^+ - X^1\Sigma_g^+$ (N ₂ ⁺)	Absorption	< 960			Rydberg series	(62.39, 43.14, 42.13, 38.10, 34.9, 30.1)
	XLVIII	$C^2\Sigma_u^+ - X^1\Sigma_g^+$ (N ₂ ⁺)	Absorption	570-470			Rydberg series	(66.60, 52.19)
	XLIX	Continuum	Absorption	1000-610				(73.151)

I. $A^3\Sigma_u^+ \leftarrow X^1\Sigma_g^+$ (Vegard-Kaplan) System

Band heads, λ (61.38, 50.17):

v', v''	2	3	4	5	6	7	8	9
0	2215.1	2332.8	2461.6	2603.6	2760.8	2935.7		3351.5
1	2146.6	2257.2	2377.5	2509.8	2655.5	2817.1	2997.0	3197.5
2		2187.8	2300.7	2424.2	2560.1	2710.1		
3		2123.5	2229.9	2346.0	2472.5	2612.8	2766.9	
4			2164.5	2274.0		2523.4	2666.6	
5				2207.2	2319.7	2441.8	2576.0	2722.5

II. $B^3\Pi_g \leftarrow X^1\Sigma_g^+$ (Wilkinson) System

Band heads: (v', v'') (0,0) (1,0)
 λ 1685 1638

III. $W^3\Delta_u \leftarrow X^1\Sigma_g^+$ (Saum-Benesch) System

Band heads, λ (70.101, 70.94):

v', v''	0	1	2	3	4	5	6	7	8
0	1683.6	1752.4	1826.0	1905.1	1990.2	2082.0	2181.4	2289.1	2406.4
1	1642.7	1708.1	1778.0	1852.9	1933.3	2019.9	2113.2	2214.2	2323.8
2	1604.4	1666.7	1733.2	1804.3	1880.4	1962.2	2050.2	2145.1	2247.7
3	1568.3	1627.8	1691.2	1758.8	1831.1	1908.5	1991.7	2081.1	2177.6
4	1534.4	1591.3	1651.8	1716.3	1785.0	1858.6	1937.3	2021.9	2112.8
5	1502.9	1557.0	1614.9	1676.4	1742.0	1811.9	1886.7	1966.8	2052.7
6	1472.8	1524.6	1580.1	1639.0	1701.6	1768.3	1839.4	1915.4	1996.9
7	1444.2	1494.1	1547.4	1603.8	1663.7	1727.4	1795.2	1867.5	1944.9
8	1416.9	1465.3	1516.5	1570.6	1628.0	1689.0	1753.7	1822.7	1896.3
9	1391.5	1438.1	1487.3	1539.4	1594.5	1652.9	1714.9	1780.8	1851.0
10	1367.3	1412.3	1459.8	1509.9	1562.8	1618.9	1678.3	1741.4	1808.5

IV. $B'^3\Sigma_u^- \leftarrow X^1\Sigma_g^+$ (Ogawa-Tanaka-Wilkinson) System

Band heads, λ (66.61, 60.35, 59.30):

v', v''	0	1	2	3	4	5	6	7	8
0	1518.1			1695.6	1762.6	1834.2		1993.0	2081.2
1	1484.4		1593.9	1653.8	1717.5			1935.4	2018.6
2	1452.8						1808.6	1881.9	
3	1422.9								
4	1394.7								
5	1368.1								
6	1342.8								
7	1318.9								
8	1296.2								
9	1274.7								
10	1254.2								

V. $a'^1\Sigma_u^- \rightleftharpoons X^1\Sigma_g^+$ (Ogawa-Tanaka-Wilkinson-Mulliken) System

Band heads in absorption, λ (Intensity) (66.61):

(v', v'')	(0, 0)	(1, 0)	(2, 0)	(3, 0)	(4, 0)	(5, 0)	(6, 0)
λ	1477.1	1446.5	1414.7	1387.6	1360.5	1335.0	1310.7
(Intensity)	(2)	(4)	(8)	(16)	(22)	(30)	(30)
(v', v'')	(7, 0)	(8, 0)	(9, 0)	(10, 0)	(11, 0)	(12, 0)	(13, 0)
λ	1287.7	1265.8	1245.0	1225.3	1206.4	1188.5	1171.3
(Intensity)	(52)	(60)	(48)	(42)	(33)	(34)	(28)
(v', v'')	(14, 0)	(15, 0)	(16, 0)	(17, 0)	(18, 0)	(19, 0)	
λ	1155.0	1139.3	1124.6	1110.0	1096.3	1083.2	
(Intensity)	(24)	(20)	(16)	(10)	(6)	(4)	

Band heads in emission, λ (Intensity) (60.33, 59.33):

(v', v'')	(0, 8)	(0, 7)	(0, 6)	(0, 5)	(0, 4)	(0, 3)
λ	2004.2	1922.2	1845.6	1774.0	1707.0	1643.8
(Intensity)	(1)	(2)	(3)	(4)	(4)	(3)

VI. $a^1\Pi_g \leftarrow X^1\Sigma_g^+$ (Lyman-Birge-Hopfield) System

Band heads in emission, λ (66.61):

v', v''	9	10	11	12	13	14	15	16	17
0									
1	1972.6								
2		1988.9	2073.0						
3			2006.0	2089.7	2181.1	2278.3			
4			1944.3	2023.5	2108.1	2198.7	2296.1		
5				1961.8	2041.2	2125.9	2216.6	2314.0	2418.4
6					1979.5	2059.0	2144.0	2234.8	2332.2
7									2253.4

VII. $w^1\Delta_u \leftarrow X^1\Sigma_g^+$ (Tanaka) System

Band heads, λ (Intensity) (64.46):

(v', v'')	(0, 0)	(1, 0)	(2, 0)	(3, 0)	(4, 0)	(5, 0)
λ	1393.9	1364.7	1337.1	1311.0	1286.3	1262.9
(Intensity)		(1)	(2)	(3)	(3)	(4)
(v', v'')	(6, 0)	(7, 0)	(8, 0)	(9, 0)	(10, 0)	(11, 0)
λ	1240.6	1219.4	1199.3	1180.3	1162.1	1144.7
(Intensity)	(5)	(7)	(6)	(6)	(5)	(4)

VIII. $C^3\Pi_u \leftarrow X^1\Sigma_g^+$ (Tanaka) System

Band heads, λ (Intensity) (66.61):

(v', v'')	(0, 0)	(1, 0)	(2, 0)
λ	1124.2	1099.6	1076.3
(Intensity)	(45)	(60)	(30)

IX. $E^3\Sigma_g^+ \leftarrow X^1\Sigma_g^+$ System

Represents a part of a Rydberg series corresponding to a $N_2^+ X^2\Sigma_g^+$ core.

Band heads, λ (74.188, 73.166):

(v', v'')	(0, 0)	(1, 0)	(2, 0)
λ	1043.9	1020.7	998.9

X. $a''^1\Sigma_g^+ \leftarrow X^1\Sigma_g^+$ (Dressler-Lutz) System

Represents part of a Rydberg series corresponding to a $N_2^+ X^2\Sigma_g^+$ core.

Band heads, λ (67.67):

(v', v'')	$(0, 0)$	$(1, 0)$
λ	1011.5	990.9

XI. $b^1\Pi_u \leftarrow X^1\Sigma_g^+$ System

Band heads, λ (73.166, 69.83, 69.82, 69.81):

(v', v'')	λ	(v', v'')	λ
(0, 0)	991.9	(8, 0)	935.1
(1, 0)	985.6	(9, 0)	929.0
(2, 0)	978.9	(10, 0)	922.7
(3, 0)	972.1	(11, 0)	916.4
(4, 0)	965.7	(12, 0)	910.5
(5, 0)	955.1	(13, 0)	904.7
(6, 0)	949.2	(14, 0)	899.2
(7, 0)	942.4	(15, 0)	895.9

XII. $F^3\Pi_u \leftarrow X^1\Sigma_g^+$ System

Represents a part of a Rydberg series corresponding to a $N_2^+ A^2\Pi_u$ core.

Band heads, λ (73.166):

(v', v'')	$(0, 0)$	$(1, 0)$	$(2, 0)$
λ	972.2	955.0	938.4

XIII. G³Π_u ← X¹Σ_g⁺ System

Represents part of a Rydberg series corresponding to a N₂⁺ X²Σ_g⁺ core.

Band heads, λ (73.166):

(v', v'')	(0, 0)	(1, 0)
λ	967.7	949.2

XIV. D³Σ_u⁺ ← X¹Σ_g⁺ System

Represents part of a Rydberg series corresponding to a N₂⁺ X²Σ_g⁺ core.

Band head, λ (73.166):

(v', v'')	(0, 0)
λ	965.4

XV. b'¹Σ_u⁺ ← X¹Σ_g⁺ System

Band heads, λ (69.83, 69.82, 69.81, 64.47):

(v', v'')	λ	(v', v'')	λ
(0, 0)	964.6	(8, 0)	-
(1, 0)	957.7	(9, 0)	907.5
(2, 0)	951.0	(10, 0)	901.4
(3, 0)	944.6	(11, 0)	896.2
(4, 0)	937.9	(12, 0)	891.0
(5, 0)	931.9	(13, 0)	885.7
(6, 0)	926.1	(14, 0)	880.7
(7, 0)	917.8	(15, 0)	875.9

XVI. c¹Π_u ← X¹Σ_g⁺ System

c₃ represents the first member of a Rydberg series corresponding to a N₂⁺ X²Σ_g⁺ core.

Band heads, λ (69.83, 69.82, 69.81, 64.47):

(v', v')	λ
(0, 0)	960.3
(1, 0)	920.0

XVII. $c'_1 \Sigma_u^+ \leftarrow X^1 \Sigma_g^+$ System

c_4' represents the first member of a Rydberg series corresponding to a $N_2^+ X^2 \Sigma_g^+$ core.

Band heads, λ (69.83, 69.82, 69.81, 64.47):

(v', v'')	λ	(v', v'')	λ
(0, 0)	958.6	(4, 0)	886.8
(1, 0)	940.1	(5, 0)	870.8
(2, 0)	921.2	(6, 0)	856.0
(3, 0)	903.7	(7, 0)	841.9

XVIII. $o^1 \Pi_u \leftarrow X^1 \Sigma_g^+$ System

Represents the first member of the Worley Rydberg series corresponding to a $N_2^+ A^2 \Pi_u$ core.

Band heads, λ (69.83, 69.82, 69.81, 64.47):	(v', v'')	λ
	(0, 0)	946.1
	(1, 0)	928.9
	(2, 0)	912.6
	(3, 0)	897.2
	(4, 0)	882.5

XIX. $e^1 \Pi_u \leftarrow X^1 \Sigma_g^+$ System

e_4 represents a member of the Worley-Jenkins Rydberg series corresponding to a $N_2^+ X^2 \Sigma_g^+$ core.

Band heads, λ (69.90):

(v', v'')	(0, 0)	(1, 0)	(2, 0)
λ	865.1	849.9	834.2

XX. $e'_1 \Sigma_u^+ \leftarrow X^1 \Sigma_g^+$ System

e_4' represents a member of the Worley-Jenkins Rydberg series corresponding to a $N_2^+ X^2 \Sigma_g^+$ core.

Band head, λ (69.90):	(v', v'')	(0, 0)
	λ	863.8

XXI. $B^3\Pi_g \rightarrow A^3\Sigma_u^+$ (First Positive) SystemBand heads, λ (Intensity) (50.17):

v', v''	0	1	2	3	4	5	6
0	10510.0(10)						
1	8912.4(10)						
2	7753.2(6)	8722.3(8)	9942.0(2)				
3	6875.0(2)	7626.2(7)	8541.8(6)	9682.1(3)			
4	6186.8(3)	6788.6(6)	7503.9(7)	8369.2(2)	9436.4(3)		
5	5632.7(1)	6127.4(3)	6704.8(8)	7386.6(5)	8204.8(3)	9203.9(2)	
6		5592.9(1)	6069.7(7)	6623.6(9)	7273.3(3)	8047.4(2)	
7			5553.7(1)	6013.6(7)	6544.8(10)	7164.8(2)	7896.4(2)
8				5515.6(2)	5959.0(8)	6468.5(10)	7059.0(2)
9					5478.5(2)	5906.0(8)	6394.7(9)
10						5442.3(3)	5854.4(8)
11						5053.6	5407.1(3)
12							5030.8

XXII. $E^3\Sigma_g^+ \rightarrow A^3\Sigma_u^+$ (Herman-Kaplan) SystemBand heads, λ (74.188, 45.16, 35.9):

v', v''	0	1	2	3	4	5	6	7
0		2242.3	2315.3	2391.6	2471.4	2554.9	2642.1	2733.2
1		2137.6	2203.8	2272.9		2419.8	2497.8	

XXIII. $W^3\Delta_u \approx B^3\Pi_g$ (Wu-Benesch) SystemBand heads, λ (n.p. 218, 71.101, 70.92, 68.73):

v', v''	0	1	2	3	4	5	6
0	629373.3	-65875.5	-31578.9	-20889.5	-15675.8	-12589.4	-10549.8
1	61962.2	586939.5	-58422.4	-30011.2	-20307.6	-15412.6	-12462.8
2	32833.3	73057.5	-357305.2	-52623.6	-28633.1	-19777.0	-15169.8
3	22450.3	36005.1	88595.4	-203381.4	-47987.9	-27413.9	-19292.1
4	17124.2	24002.4	39775.2	111892.7	-143172.7	-44201.2	-26329.2
5	13885.3	18099.6	25797.6	44328.0	150660.7	-111088.6	-41053.2
6	11708.4	14568.8	19174.3	27817.1	49931.5	227885.3	-91169.0
7	10145.4	12225.3	15311.3	20363.6	30133.7	56992.5	456755.3
8	8969.2	10557.0	12781.6	16120.4	21686.6	32816.8	66157.9
9	8052.4	9309.4	10997.3	13382.0	17005.2	23166.3	35959.1
10	7318.0	8341.7	9671.8	11469.3	14051.7	17976.5	24831.6

XXIV. $B'^3\Sigma_u^- \rightarrow B^3\Pi_g$ ("Y" Bands) SystemBand heads, λ (Intensity) (50.17):

v', v''	0	1	2	3	4
4	8058(2)				
5	7243(2)	8262(5)			
6	6587(1)	7420(6)	8473(8)		
7	6062(1)	6744(6)	7602(10)	8691(10)	
8		6203(3)	6905(10)	7791(10)	8917(2)

XXV. $C^3\Pi_u \rightarrow B^3\Pi_g$ (Second Positive) SystemBand heads, λ (Intensity) (50.17):

v', v''	0	1	2	3	4	5
0	3371.3(10)	3576.9(10)	3804.9(10)	4059.4(8)	4343.6(4)	4667.3(0)
1	3159.3(9)	3338.9(2)	3536.7(8)	3755.4(10)	3998.4(9)	4269.7(5)
2	2976.8(6)	3136.0(8)	3309 (2)	3500.5(4)	3710.5(8)	3943.0(8)
3	2819.8(1)	2962.0(6)	3116.7(6)	3285.3(3)	3469 (0)	3671.9(6)
4	2687	2814.3(1)	2953.2(6)	3104.0(3)	3268.1(4)	3446 (0)

XXVI. $C'^3\Pi_u \rightarrow B^3\Pi_g$ (Goldstein-Kaplan) SystemBand heads, λ (50.17):

v', v''	2	3	4	5	6	7	8	9	10
0	2863.5	3005.4	3159.2	3326.1	3504.0	3707.1	3925.4	4166.0	4432.2
1			3025.8	3178.4					

XXVII. $D^3\Sigma_u^+ \rightarrow B^3\Pi_g$ (Fourth Positive) SystemBand heads, λ (Intensity) (50.17):

(v', v'')	(0, 6)	(0, 5)	(0, 4)	(0, 3)	(0, 2)	(0, 1)	(0, 0)
λ	2903.9	2777.9	2660.5	2550.7	2448.0	2351.4	2260.8
(Intensity)	(1)	(2)	(5)	(8)	(10)	(6)	(2)

XXVIII. $E^3\Sigma_g^+ \rightarrow B^3\Pi_g$ SystemBand heads, λ (69.88):

(v', v'') λ	(0,0)	(0,1)	(0,2)	(0,3)
	2740	2880	3020	3180

XXIX. $a^1\Pi_g \rightarrow a'^1\Sigma_u^-$ (MacFarlane Infrared) System

Band heads, λ (65.58):

(v', v'') λ	(0,0)	(1,0)	(2,1)
	82439.2	34739.4	33214.5

XXX. $x^1\Sigma_g^- \rightarrow a'^1\Sigma_u^-$ (Fifth Positive) SystemBand heads, λ (Intensity) (50.17):

v', v''	0	1	2	3	4	5	6
0	2198.9(4)	2274.3(6)	2353.6(4)		2525.6(2)	2619.3(4)	
1	2112.1(5)	2181.5(4)		2331.3(2)	2411.8(7)	2496.7(3)	2586.6(7)
2	2033.6(5)	2097.9(2)	2165.2(5)	2235.9(3)		2387.9	2469.9(4)

XXXI. $y^1\Pi_g \rightarrow a'^1\Sigma_u^-$ (First Kaplan) SystemBand heads, λ (Intensity) (50.17):

v', v''	0	1	2	3	4
0	2153.6(4)	2225.9(5)	2301.9(4)	2381.7(3)	2466.0(2)
1	2077.3			2288.6(1)	2366.4(2)

XXXII. $w^1\Delta_u \rightarrow a^1\Pi_g$ (MacFarlane Infrared) System

Band head, λ (66.64):

(v', v'') λ	(0,0)
	36399.5

XXXIII. $b^1\Pi_u \rightarrow a^1\Pi_g$ (Gaydon-Herman) System

Band heads, λ (69.82, 69.81, 57.27):

v', v''	0	1	2	3	4
0					
1	3075.1	3241.3			
...					
5	2795.4	2932.0	3079.9	3240.8	3416.5
6	2746.2	2877.9	3020.3	3175.0	

XXXIV. $b'^1\Sigma_g^+ \rightarrow a^1\Pi_g$ (Gaydon-Herman) System

Band head, λ (69.82, 69.81, 57.27): (v', v'') $(0, 7)$
 λ 2498.6

XXXV. $c^1\Pi_u \rightarrow a^1\Pi_g$ (Gaydon-Herman) System

c_3 and c_4 are the two first members of a $c^1\Pi_u$ Rydberg series that converges at $N_2^+ X^2\Sigma_g^+$.

Band heads, λ (69.82, 69.81, 57.27):

$c_3^1\Pi_u \rightarrow a^1\Pi_g$

v', v''	0	1	2	3	4
0	2839.4	2980.1			
1					
2	2516.0	2626.2	2744.3	2871.1	3008.1

$c_4^1\Pi_u \rightarrow a^1\Pi_g$

v', v''	0	1	2	3	4	5	6
0		2224.4	2308.6	2397.8	2492.4	2592.8	2699.9

XXXVI. $c'^1\Sigma_u^+ \rightarrow a'^1\Pi_g$ (Gaydon-Herman) System

c_4' is the first member of a $c'^1\Sigma_u^+$ Rydberg series that converges at $N_2^+ X^2\Sigma_g^+$.

Band heads, λ (69.82, 69.81, 57.27):

v', v''	0	1	2	3	4	5
0	2827.1	2967.0	3118.6	3283.3	3463.3	3661.1
1	2671.7	2796.0				
2	2524.9		2753.8			
3	2397.1	2496.8	2603.3			
4	2281.5	2371.6	2467.7	2569.6	2678.5	2795.6

XXXVII. $d'(^1\Sigma_u^- \text{ or } ^1\Delta_u?) \rightarrow a'^1\Pi_g$ (Gaydon-Herman) System

Band heads, λ (69.82, 69.81, 57.27):

v', v''	0	1	2
0	2358.8	2455.1	2558

XXXVIII. $o'^1\Pi_u \rightarrow a'^1\Pi_g$ (Gaydon-Herman) System

o is the first member of the Worley Rydberg series that converges at $N_2^+ A^2\Pi_u$.

Band heads, λ (69.82, 69.81, 57.27):

(v', v'')	(0, 0)	(0, 1)
λ	2723.6	2853.3

XXXIX. $y'^1\Pi_g \rightarrow w'^1\Delta_u$ (Seconu Kaplan) System

Band heads, λ (Intensity) (50.17):

v', v''	0	1	2	3	4	5	6
0	2354.5(4)		2536.6(5)	2636.2(5)	2741.9(3)	2854.9	
1	2263.4(4)		2431.0	2522.3(3)	2619.3(5)	2722.0(3)	2831.7

XL. $z^1\Delta_g \rightarrow w^1\Delta_u$ System

Band heads, λ (57.27): (v', v'') $(n, 2)$ $(n+3, 4)$ for $n=2?$
 λ 2477.3 2368.8

XLI. $E^3\Sigma_g^+ \rightarrow C^3\Pi_u$ System

Band head, λ (69.88): (v', v'') (0, 0)
 λ 12843.6

XLII. Gaydon Green System

Band heads, λ (54.23, 53.22, 44.15):

v', v''	0	1	2	3	4	5
0	5574.4(9)	5815.1(10)	6068.6(8)	6336.3(5)		
1	5308.6(8)	5527.1(2)	5755.1(3)	5994.5(6)	6246.3(5)	
2	5073.4(4)	5272.0(5)	5479.6(6)		5924 (1)	6160.5(3)
3		5047.0(2)		5435.0(3)	5640 (1)	

XLIII. Herman Infrared System

Band heads, λ (53.22, 51.18):

v', v''	0	1	2
0	8057.6(10)	8549 (2)	
1	7521.0(0)		8397 (1)
2	7061.7(6)	7435.0(5)	7828.5(8)
3		7001.2(4)	

XLIV. $X^2\Sigma_g^+(N_2^+) \leftarrow X^1\Sigma_g^+$ (Worley-Jenkins) System

Represents a $^1\Pi_u$ Rydberg series, the first state of which is $c^1\Pi_u$
 (69.82, 69.81, 67.66, 62.39)

$$\nu = 125665.8 - R \left[m + 0.3450 - (0.1000/m) - (0.100/m^2) \right]^{-2}$$

where $m = 2, 3, \dots 26$

XLV. $X^2\Sigma_g^+(N_2^+) \leftarrow X^1\Sigma_g^+$ (Carroll-Yoshino) System

Represents a $^1\Sigma_u^+$ Rydberg series, the first member of which is $c' ^1\Sigma_u^+$ (69.82, 69.81, 67.66)

m	2	3	4	5	6	7
λ	958.559	(863.6)	833.746	820.592	(813.2)	808.672
n*	2.2675		4.3776	5.3713		7.394

XLVI. $A^2\Pi_u(N_2^+) \leftarrow X^1\Sigma_g^+$ (Worley) System

Represents a $^1\Pi_u$ Rydberg series, the first of which is $o ^1\Pi_u$ (62.39, 53.21, 53.20)

$$v = 136607 - R \left[m - 0.0441 - (0.018/m^2) \right]^{-2} \text{ where } m = 2, 3, \dots 6$$

XLVII. $B^2\Sigma_u^+(N_2^+) \leftarrow X^1\Sigma_g^+$ (Hopfield) System

Represents a Rydberg series (62.39, 43.14, 42.13, 38.10, 24.8, 30.1)

$$v = 151240 - R(m - 0.092)^{-2} \text{ where } m = 3, 4, \dots 7$$

XLVIII. $C^2\Sigma_u^+(N_2^+) \leftarrow X^1\Sigma_g^+$ System

Represents a Rydberg series

Band heads, λ (66.60, 52.19):

n* = 3.040	(v', v'')	λ	(v', v'')	λ
	(0, 0)	560.48	(7, 0)	520.46
	(1, 0)	554.10	(8, 0)	515.61
	(2, 0)	548.00	(9, 0)	510.93
	(3, 0)	542.11	(10, 0)	506.35
	(4, 0)	536.41	(11, 0)	502.02
	(5, 0)	530.86	(12, 0)	497.77
	(6, 0)	525.54	(13, 0)	493.71

$n^* = 4.059$	(v', v'')	λ
	(3, 0)	527.33
	(4, 0)	521.89
	(5, 0)	516.71
	(6, 0)	
	(7, 0)	506.71
	(8, 0)	502.02

$n^* = 5.05$	(v', v'')	λ
	(8, 0)	496.15

XLIX. Continuum

There are two weak continua between 825 and 1000 Å with maximums of approximately 5 cm^{-1} at 970 Å and 15 cm^{-1} at 910 Å. At approximately 850 Å a dissociation continuum increases gradually to a maximum of $\sim 120 \text{ cm}^{-1}$ at 805 Å. This is followed by a secondary peak with a maximum value of 75 cm^{-1} occurring at 775 Å. The continuum then decreases to 0 at $\sim 750 \text{ Å}$. The most prominent dissociation continuum starts at approximately 730 Å and decreases to 90 cm^{-1} at 660 Å. Below 660 Å there is another continuum with a broad maximum at 610 Å, this continuum overlapping the previous one. (73.151)

SPECTROSCOPIC CONSTANTS

Molecule N₂

State	T ₀	ω_e	$\times_e \omega_e$	B _e	$\alpha_e \times 10^3$	D _e × 10 ⁶	r _e	Remarks	Bibliography
e' ¹ Σ _u ⁺	115767.5							Rydberg	(69.90)
e' ¹ Π _u	115593.6							Rydberg	(69.90)
z' ¹ Δ _g	115365.9	(1700)		(1.76)	15.3		(1.16)	Rydberg	(57.27)
y' ¹ Π _g	114166.3	^(a) 1707.9		1.78 ^(b)			1.16 ^(c)	Rydberg	(57.28)
x' ¹ Σ _g ⁻	113212.1	1910.0		1.750	22.5	5.88	1.168	Rydberg	(56.26)
d' ¹ ? _u	111333								(45.16)
o' ¹ Π _u	105682	2020.0	32.28	1.694 ^(b)			1.19 ^(c)	Rydberg	(69.82, 69.81)
c' ¹ Σ _u ⁺	104322.4	2046 ^(a)		1.929 ^(b)			1.12 ^(c)	Rydberg	(69.82, 69.81)
c' ¹ Π _u	104139.2	2410 ^(a)		1.50 ^(b)			1.27 ^(c)	Rydberg	(69.82, 69.81)
b' ¹ Σ _u ⁺	103672	746 ^(a)		1.154	4.8		1.444		(69.82, 69.81)
D' ³ Σ _u ⁺	103573			1.961 ^(b)		20	1.108 ^(c)	Rydberg	(40.11)

SPECTROSCOPIC CONSTANTS

State	T_0	ω_e	$\times \omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$G^3\Pi_u$	103338							Rydberg	(73.166)
$F^3\Pi_u$	102854							Rydberg	(73.166)
$b^1\Pi_u$	100816	635(a)		1.448(b)	4.8	29	1.230 ^(c)		(69.86, 69.81)
$a''^1\Sigma_g^+$	99032							Rydberg	(67.67)
$C'^3\Pi_u$	97580			1.0496(b)		10.9	1.508 ^(c)		(63.44)
$E^3\Sigma_g^+$	95774.50	2185(a)		1.927(b)		6.0	1.117 ^(c)	Rydberg	(74.188, 54.50)
$C^3\Pi_u$	88977.9	2047.18	28.4450	1.82473	18.683	5.80	1.1487		(65.50)
$5\Sigma^-$	77925	650				0.0011	1.55		(62.41)
$w^1\Delta_u$	71698.8	1559.24	11.8874	1.498	16.6	5.53	1.2678		(65.50)
$a^1\Pi_g$	68951.2	1694.20	13.9491	1.61688	17.933	5.89	1.2203		(65.50)
$a'^1\Sigma_u^-$	67739.3	1530.25	12.0747	1.47988	16.574	5.54	1.2755		(65.50)

SPECTROSCOPIC CONSTANTS

State	T_0	ω_e	$\times_e \omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$B^1\ ^3\Sigma_u^-$	65852.4	1516.88	12.1810	1.47359	16.861	5.56	1.2782		(65.50)
$W^3\ \Delta_u$	60555.8	1501.4	11.6				1.28		(71.101, 65.50)
$B^3\ \Pi_g$	59306.8	1733.39	14.1221	1.6374	17.91	5.84	1.2126		(65.50)
$A^3\ \Sigma_u^+$	49754.8	1460.52	13.8313	1.45455	18.009	5.77	1.2866		(65.50)
$X^1\ \Sigma_g^+$	0	2358.03	14.1351	1.9980	17.72	5.74	1.0977		(65.50)
<p>(a) ΔG_0, (b) B_0, (c) r_0</p> <p>Dissociation energy = 9.76 ± 0.01 eV, 225.07 kcal/mole, 78710 cm^{-1} (63.43, 56.24).</p>									

Perturbations and General Information

The $D^3\Sigma_u^+$ state is predissociated by the shallow $C^3\Pi_u$ state (74.188).

The $b^1\Pi_u$ state is perturbed by the $c^1\Pi_u$ state
 The $b^1\Sigma_u^+$ state is perturbed by the $c^1\Sigma_u^+$ state } (73.166)

The $o^1\Pi_u$ level is predissociated possibly by the $C^3\Pi_u$ state (73.166).

The $B^3\Pi_g$ ($v' \sim 12$) and a $^1\Pi_g$ ($v' \sim 6$) levels are predissociated by the $^5\Sigma^+$ level (68.80).

The higher levels of the $C^3\Pi_u$ and $C^1\Pi_u$ states are predissociated by the $^3\Pi_u$ continuum (69.82).

Perturbations and predissociation have been observed in the γ state (57.28).

Lifetimes:

$A^3\Sigma_u^+$	$v' = 0$	$\tau = 1.36 \pm 0.27$ sec for $\Sigma = 0$ substate levels (69.L2, 69.L3) $\tau = 2.70 \pm 0.54$ sec for $\Sigma = 1, -1$ substate levels	
$B^3\Pi_g$	$v' = 0$	$\tau = 10 \pm 2$ μ sec	(n.p. 217)
	$v' = 2$	$\tau = 7.0 \pm 0.4$ μ sec	(66.L1)
	$v' = 3$	$\tau = 6.8 \pm 0.3$ μ sec	
	$v' = 4$	$\tau = 6.7 \pm 0.7$ μ sec	
	$v' = 5$	$\tau = 6.7 \pm 1.0$ μ sec	
	$v' = 6$	$\tau = 7.0 \pm 0.7$ μ sec	
	$v' = 7$	$\tau = 5.4 \pm 0.8$ μ sec	
	$v' = 8$	$\tau = 5.4 \pm 0.8$ μ sec	
	$v' = 9$	$\tau = 5.4 \pm 0.5$ μ sec	
$W^3\Delta_u$	$v' = 0$	$\tau = 1.668$ msec	(73.167)
	$v' = 1$	$\tau = 2.000$ msec	
$a^1\Pi_g$	$v' = 0$	$\tau = 0.17$ msec	(65.52)
$C^3\Pi_u$	$v' = 0$	$\tau = 40.4 \pm 0.5$ nsec	(73.177)
	$v' = 1$	$\tau = 40.6 \pm 0.5$ nsec	
$D^3\Sigma_u^+$	$v' = 0$	$\tau = 14.1$ nsec	(73.182)

Oscillator Strengths:

$$A^3\Sigma_u^+ \leftarrow X^1\Sigma_g^+ \quad f_{0,0} = 2 \times 10^{-3} \quad (66.L1)$$

$$a^1\Pi_g \leftarrow X^1\Sigma_g^+ \quad \begin{aligned} f_{0,0} &= 1.3 \times 10^{-6} \\ f_{1,0} &= 3.0 \times 10^{-6} \\ f_{2,0} &= 4.1 \times 10^{-6} \end{aligned} \quad (67.68)$$

$$C^3\Pi_u \leftarrow X^1\Sigma_g^+ \quad \begin{aligned} f_{0,0} &= 2.2 \times 10^{-6} \\ f_{1,0} &= 1.1 \times 10^{-6} \\ f_{2,0} &= 5.6 \times 10^{-7} \end{aligned}$$

$$w^1\Delta_u \leftarrow X^1\Sigma_g^+ \quad \left. \begin{aligned} f_{3,0} &= (3.5 + 0.18p) \times 10^{-8} \\ f_{4,0} &= (6.1 + 0.21p) \times 10^{-8} \\ f_{5,0} &= (4.0 + 0.26p) \times 10^{-8} \end{aligned} \right\} \text{ for pressure } p \text{ in psi}$$

Franck-Condon factors for the $C^3\Pi_u - B^3\Pi_g$ (Second Positive) system (65.52):

v'', v'	0	1	2	3	4
0	4.55-1	3.88-1	1.34-1	2.16-2	1.16-3
1	3.31-1	2.29-2	3.35-1	2.52-1	5.66-2
2	1.45-1	2.12-1	2.30-2	2.04-1	3.26-1
3	4.94-2	2.02-1	6.91-2	8.81-2	1.13-1
4	1.45-2	1.09-1	1.69-1	6.56-3	1.16-1
5	3.87-3	4.43-2	1.41-1	1.02-1	2.45-3
6	9.68-4	1.52-2	7.72-2	1.37-1	4.70-2
7	2.31-4	4.68-3	3.32-2	9.93-2	1.09-1
8	5.36-5	1.33-3	1.23-2	5.26-2	1.04-1
9	1.21-5	3.57-4	4.12-3	2.31-2	6.67-2
10	2.61-6	9.15-5	1.27-3	8.95-3	3.40-2

Franck-Condon factors followed by a factor of ten

Franck-Condon factors for the $B^3\Pi_g - A^3\Sigma_g^+$ (First Positive) system (65.52):

v'', v'	0	1	2	3	4	5	6	7	8
0	4.06-1	4.01-1	1.58-1	3.17-2	3.47-3	2.01-4	5.72-6	8.81-8	8.28-11
1	3.27-1	3.71-3	2.85-1	2.77-1	9.18-2	1.41-2	1.07-3	3.70-5	5.14-7
2	1.64-1	1.59-1	6.59-2	1.05-1	3.06-1	1.63-1	3.41-2	3.26-3	1.35-4
3	6.67-2	1.93-1	2.25-2	1.50-1	1.11-2	2.59-1	2.26-2	6.36-2	7.50-3
4	2.44-2	1.29-1	1.22-1	4.67-3	1.53-1	6.94-3	1.76-1	2.68-1	1.01-1
5	8.38-3	6.57-2	1.39-1	4.09-2	4.94-2	1.00-1	5.05-2	9.30-2	2.83-1
6	2.80-3	2.92-2	9.94-2	1.03-1	2.04-3	9.29-2	4.02-2	9.90-2	3.20-2
7	9.26-4	1.20-2	5.66-2	1.08-1	5.13-2	8.81-3	1.04-1	5.00-3	1.26-1
8	3.07-4	4.73-3	2.83-2	7.88-2	8.85-2	1.22-2	3.92-2	8.29-2	2.75-3
9	1.03-4	1.83-3	1.31-2	4.78-2	8.58-2	5.37-2	4.73-5	6.71-2	4.68-2

Franck-Condon factors followed by factor of ten

Franck-Condon factors for the $A^3\Sigma_u^+ - X^1\Sigma_g^+$ (Vegard-Kaplan) system (65.52):

v'', v'	0	1	2	3	4	5	6	7	8
0	1.06-3	5.55-3	1.57-2	3.15-2	5.07-2	6.93-2	8.38-2	9.21-2	9.38-2
1	8.41-3	3.27-2	6.65-2	9.31-2	9.91-2	8.35-2	5.57-2	2.78-2	8.41-3
2	3.34-2	8.88-2	1.15-1	8.91-2	4.00-2	5.73-3	1.92-3	1.90-2	3.87-2
3	8.29-2	1.33-1	8.12-2	1.35-2	3.65-3	3.44-2	5.52-2	4.64-2	2.21-2
4	1.44-1	1.09-1	9.45-3	1.74-2	6.05-2	5.16-2	1.45-2	1.60-4	1.52-2
5	1.89-1	3.67-2	1.77-2	7.36-2	3.88-2	4.23-4	1.88-2	4.41-2	3.63-2
6	1.92-1	8.43-5	8.13-2	4.21-2	1.05-2	4.10-2	4.70-2	1.23-2	1.06-3
7	1.55-1	4.26-2	7.92-2	1.22-4	5.28-2	4.21-2	8.71-4	1.90-2	4.11-2
8	1.02-1	1.17-1	1.76-2	4.83-2	5.01-2	5.30-5	3.71-2	4.04-2	5.56-3
9	5.47-2	1.53-1	6.52-3	8.10-2	8.41-4	4.56-2	3.70-2	8.28-6	2.58-2
10	2.46-2	1.32-1	7.06-2	3.10-2	3.70-2	4.73-2	5.09-4	4.04-2	3.06-2

Franck-Condon factors followed by factor of ten

Franck-Condon factors for the $a^1\Pi_g - X^1\Sigma_g^+$ (Lyman-Birge-Hopfield) system (65.52):

v'', v'	0	1	2	3	4	5	6
0	4.43-2	1.18-1	1.73-1	1.85-1	1.60-1	1.20-1	8.08-2
1	1.51-1	1.90-1	9.44-2	1.15-2	6.67-3	4.75-2	8.52-2
2	2.50-1	8.02-2	3.30-3	7.51-2	9.62-2	4.70-2	4.94-3
3	2.53-1	5.84-4	1.08-1	6.81-2	4.43-4	3.47-2	7.32-2
4	1.73-1	9.22-2	8.41-2	4.39-3	7.81-2	5.51-2	2.37-3
5	8.61-2	1.91-1	3.19-4	9.76-2	3.47-2	9.80-3	6.39-2
6	3.22-2	1.76-1	7.30-2	6.18-2	2.05-2	7.84-2	1.24-2
7	9.17-3	9.93-2	1.73-1	1.17-3	9.90-2	5.16-3	4.47-2
8	1.99-3	3.87-2	1.60-1	9.17-2	2.93-2	5.50-2	5.01-2
9	3.37-4	1.10-2	8.76-2	1.71-1	1.64-2	8.17-2	5.19-3
10	4.75-5	2.33-3	3.23-2	1.38-1	1.25-1	3.08-3	8.54-2

Franck-Condon factors followed by a factor of ten

Franck-Condon factors for the $C^3\Pi_u - X^1\Sigma_g^+$ (Tanaka) system (65.52):

v'', v'	0	1	2	3	4
0	5.50-1	3.03-1	1.01-1	2.76-2	7.16-3
1	3.36-1	8.73-2	2.71-1	1.82-1	7.88-2
2	9.03-2	3.64-1	1.82-3	1.30-1	1.82-1
3	1.33-2	1.95-1	2.44-1	7.11-2	2.42-2
4	1.12-3	4.47-2	2.67-1	9.92-2	1.48-1
5	6.28-5	5.84-3	9.52-2	2.80-1	9.47-3
6	6.12-6	5.13-4	1.80-2	1.58-1	2.19-1
7	6.77-7	4.90-5	2.27-3	4.32-2	2.13-1
8	4.83-9	5.17-6	2.79-4	8.06-3	8.76-2
9	1.44-10	1.48-7	4.21-5	1.39-3	2.40-2
10	1.68-8	9.72-8	4.41-6	2.59-4	5.66-3

Franck-Condon factors followed by factor of ten

Franck-Condon factors for the $W^3\Delta_u - X^1\Sigma_g^+$ system (70.94):

v', v''	0	1	2	3	4	5	6	7
0	.1713-2	.1310-1	.4721-1	.1065-6	.1691-0	.2005-0	.1846-0	.1354-0
1	.8568-2	.4711-1	.1107-0	.1384-0	.8733-1	.1401-1	.9521-2	.7826-1
2	.2295-1	.8741-1	.1204-0	.5727-1	.1253-3	.4533-1	.9516-1	.5355-1
3	.4383-1	.1099-0	.7206-1	.1040-2	.4385-1	.7576-1	.1548-1	.1425-1
4	.6680-1	.1025-0	.1818-1	.2143-1	.6970-1	.1385-1	.1912-1	.6786-1
5	.8696-1	.7284-1	.7807-4	.5735-1	.3075-1	.7809-2	.5891-1	.1536-1
6	.1003-0	.3743-1	.1649-1	.5698-1	.5108-3	.4486-1	.2615-1	.8806-2
7	.1050-0	.1106-1	.4202-1	.2820-1	.1368-1	.4519-1	.2614-4	.4465-1
8	.1021-0	.3046-3	.5511-1	.4007-2	.3909-1	.1477-1	.2141-1	.3225-1
9	.9325-1	.3737-2	.4992-1	.1816-2	.4350-1	.1630-4	.4062-1	.2814-2
10	.8129-1	.1581-1	.3329-1	.1623-1	.2659-1	.1279-1	.2831-1	.6968-2

Franck-Condon factors followed by a factor of ten

r-Centroids for the $B^3\Sigma_u^- - X^1\Sigma_g^+$ system (66.65a).

v', v''	0	1	2	3	4	5	6	7	8
0	1.182	1.199	1.216	1.234	1.252	1.271	1.290	1.310	1.330
1	1.171	1.188	1.205	1.222	1.240	1.258	1.277	1.296	1.316
2	1.161	1.177	1.194	1.211	1.228	1.246	1.264	1.283	1.302
3	1.151	1.167	1.183	1.200	1.217	1.234	1.252	1.270	1.289

Lasing from the First Positive system has been observed (n.p. 217, 67.68a, 63.43a).

Lasing from the Second Positive system has been observed (n.p. 217, 74.206, 74.204, 74.199, 74.197, 74.195, 74.193, 74.191, 74.190, 74.189, 73.168, 73.165, 73.163, 68.74a, 67.68a, 66.64a, 64.47a).

Lasing from the Lyman-Birge-Hopfield system has been observed (73.168).

The two MacFarlane infrared systems have only been seen in lasing (n.p. 217 66.65, 66.63a, 65.58).

BIBLIOGRAPHY

The references for this molecule are only those from which spectroscopic information has been taken directly and those papers published after 1967. An excellent bibliography is given in reference (68.80) that provides a listing through 1967 as well as a review of reactions of the N₂ molecule.

- (30. 1) Hopfield Rydberg Series,
J. J. Hopfield,
Phys. Rev. 36, 789
- (30. 2) F. Charola,
Phys. Z. 31, 457-63
- (32. 3) Vegard-Kaplan System,
L. Vegard,
Z. Physik 75, 30-62
- (34. 4) First and Second Goldstein-Kaplan Systems,
J. Kaplan,
Phys. Rev. 46, 534
- (34. 5) First and Second Goldstein-Kaplan Systems,
J. Kaplan,
Phys. Rev. 46, 534
- (34. 6) First and Second Goldstein-Kaplan Systems,
J. Kaplan,
Phys. Rev. 46, 631
- (34. 7) W. W. Lozier,
Phys. Rev. 45, 752
- (34. 8) Hopfield Rydberg Series,
R. S. Mulliken,
Phys. Rev. 46, 144-6
- (35. 9) First and Second Herman-Kaplan and Kaplan Systems,
J. Kaplan,
Phys. Rev. 47, 259
- (38. 10) Hopfield Rydberg Series,
T. Takamine, T. Suga, and Y. Tanaka,
Sci. Papers Inst. Phys. Chem. Res. 34, 854-64

- (40. 11) Fourth Positive System,
L. Gerö and R. Schmid,
Z. Physik 116, 589-603
- (42. 12) N. M. Emanuel,
C. R. Acad. Sci. 36, 145-9
- (42. 13) Worley-Jenkins Rydberg Series,
Y. Tanaka and T. Takamine,
Sci. Papers Inst. Phys. Chem. Res. 39, 427-36
- (43. 14) Worley Rydberg Series,
R. E. Worley,
Phys. Rev. 64, 207-24
- (44. 15) Gaydon Green System,
A. G. Gaydon,
Proc. Phys. Soc. 56, 85-95
- (45. 16) Gaydon-Herman and Herman-Kaplan Systems. Predissociation of
the a State,
R. Herman-Montagne,
Ann. Phys. 20, 241-91
- (50. 17) Tables of Band Heads,
R. W. B. Pearse and A. G. Gaydon,
Identification of Molecular Spectra
2nd Edition, Chapman & Hall, London
- (51. 18) Herman Infrared System,
R. Herman,
C. R. Acad. Sci. 233, 733-40
- (52. 19) Rydberg Series,
G. L. Weissler, P. Lee, and E. I. Mohr,
J. Opt. Soc. Am. 42, 84-90
- (53. 20) Worley Rydberg Series,
R. E. Worley,
Phys. Rev. 89, 863-4
- (53. 21) Rydberg Series,
R. E. Worley,
Phys. Rev. 90, 1131
- (53. 22) Fifth Positive, Gaydon Green, and Herman Infrared Systems,
P. K. Carroll and N. D. Sayers,
Proc. Phys. Soc. A 66, 1138-44

- (54. 23) Gaydon Green System,
A. E. Grün,
Z. Naturforsch. A 9, 1017-9
- (56. 24) Dissociation Energy,
L. Brewer and A. W. Searcy,
Ann. Rev. Phys. Chem. 7, 259-86
- (56. 25) Lyman-Birge-Hopfield System in Emission,
A. Lofthus,
Can. J. Phys. 34, 780-9
- (56. 26) Fifth Positive System,
A. Lofthus,
J. Chem. Phys. 25, 4^o4-7
- (57. 27) Gaydon-Herman, Z - W Systems,
A. Lofthus,
Can. J. Phys. 35, 216-34
- (57. 28) First and Second Kaplan Systems. Perturbations and Predissociations in the γ State,
A. Lofthus and R. S. Mulliken,
J. Chem. Phys. 27, 1010-7
- (58. 29) $B' - B$ System,
F. LeFlanc, Y. Tanaka, and A. Jursa,
J. Chem. Phys. 28, 979-81
- (59. 30) $a' - X$ and $B' - X$ Systems,
M. Ogawa and Y. Tanaka,
J. Chem. Phys. 30, 1354-5
- (59. 31) Vegard-Kaplan System in Absorption,
P. G. Wilkinson,
J. Chem. Phys. 30, 773-6
- (59. 32) $a' - X$ System,
P. G. Wilkinson and R. S. Mulliken,
J. Chem. Phys. 31, 674-9
- (59. 33) First and Second Positive Systems. A Doubling and Triplet Separations in the B Perturbations,
G. H. Dieke and D. F. Heath,
U. S. Dept. Com., Office Tech. Serv., PB 146.250

- (60. 34) B' - B System Rotational Analysis,
G.H. Dieke and D. F. Heath,
J. Chem. Phys. 33, 432-6
- (60. 35) a' - X, B' - X Systems,
M. Ogawa and Y. Tanaka,
J. Chem. Phys. 32, 754-8
- (60. 36) B' - B System. Triplet Separation in the B State,
P.K. Carroll and H. E. Rubalcava,
Proc. Phys. Soc. 76, 337-45
- (60. 37) First and Second Positive Systems,
D. F. Heath,
Los Alamos Sci. Lab. Rept., U. S. At. Energy Comm. LA-2335
- (61. 38) Persistent Aurora Spectra,
Y. Tanaka and A. S. Jursa,
J. Opt. Soc. Am. 51, 1239-45
- (62. 39) Rydberg Series,
M. Ogawa and Y. Tanaka,
Can. J. Phys. 40, 1593-607
- (62. 40) Vegard-Kaplan Systems,
N. P. Carleton and C. Papaliolios,
J. Quant. Spectrosc. Radiative Trans. 2, 241-4
- (62. 41) P. K. Carroll,
"Note on the $5\Sigma_g^+$ State of N₂,"
J. Chem. Phys. 37, 805-9²
- (62. 42) B - X System,
P. G. Wilkinson,
J. Quant. Spectrosc. Radiative Trans. 2, 343-8
- (63. 43) Dissociation and Ionization Energies,
P. G. Wilkinson,
Astrophys. J. 138, 778-800
- (63. 43a) L. E. S. Mathias and J. T. Parker,
"Stimulated Emission in the Band Spectrum of Nitrogen,"
Appl. Phys. Letters 3, 16-18
- (63. 44) Goldstein-Kaplan Systems,
P. K. Carroll,
Proc. Roy. Soc. A 272, 270-83

- (64. 45) Isotope Displacements and Vibrational Structure,
D. Mahon-Smith and P. K. Carroll,
J. Chem. Phys. 41, 1377-82
- (64. 46) Forbidden Absorption System,
Y. Tanaka, M. Ogawa, and A. S. Jursa,
J. Chem. Phys. 40, 3690-700
- (64. 47) Far Ultraviolet Spectra,
S. G. Tilford and P. G. Wilkinson,
J. Molec. Spectrosc. 12, 231-88
- (64. 47a) H. G. Heard,
"High-Power Ultraviolet Gas Laser,"
Bull. Am. Phys. Soc. 9, 65
- (64. 48) Inverse Predissociation,
S. G. Tilford and P. G. Wilkinson,
J. Molec. Spectrosc. 12, 347-59
- (64. 49) Second Positive System,
D. C. Tyte and R. W. Nicholls,
Identification Atlas of Molecular Spectra
York Univ. Center for Res. in Exp. Space Sci. and Dept. of Phys.,
Toronto, Ontario, 2
- (65. 50) Potential Energy Curves,
W. Benesch, J. T. Vanderslice, S. G. Tilford, and P. G. Wilkinson,
Astrophys. J. 142, 1227-40
- (65. 51) B' - X System. High Resolution Spectra,
S. G. Tilford, J. T. Vanderslice, and P. G. Wilkinson,
Astrophys. J. 141, 1226-65
- (65. 52) R. N. Zare, E. O. Larsson, and R. A. Berg,
"Franck-Condon Factors for Electronic Band Systems of Molecular
Nitrogen,"
J. Molec. Spectrosc. 15, 117-39
- (65. 53) C - X System. High Resolution Study,
S. G. Tilford, J. T. Vanderslice, and P. G. Wilkinson,
Astrophys. J. 142, 1203-26
- (65. 54) a' - X System. High Resolution Study,
S. G. Tilford, P. G. Wilkinson, and J. T. Vanderslice,
Astrophys. J. 141, 427-43

- (65.55) a - X System. High Resolution Study,
J. T. Vanderslice, S. G. Tilford, and P. G. Wilkinson,
Astrophys. J. 141, 395-426
- (65.56) Predissociation,
P. K. Carroll and R. S. Mulliken,
J. Chem. Phys. 43, 2170-9
- (65.57) Vegard-Kaplan System,
R. E. Miller,
J. Chem. Phys. 43, 1695-701
- (65.58) a - a' System. Laser Stimulated Transition,
R. A. MacFarlane,
Phys. Rev. A 140, 1070-1
- (65.59) Lyman-Birge-Hopfield System,
D. J. MacEwen,
Thesis, University Western Ontario
- (66.60) Photoionization,
K. Codling,
Astrophys. J. 143, 552-8
- (66.61) Vacuum Ultraviolet Absorption Spectra,
S. G. Tilford, P. G. Wilkinson, V. B. Franklin, R. H. Naber,
W. Benesch, and J. T. Vanderslice,
Astrophys. J. Suppl. 13, 31-64
- (66.62) a' - X System. Franck-Condon Factors,
K. C. Joshi,
J. Atm. Terrestr. Phys. 28, 521-5
- (66.63) A State,
R. E. Miller,
J. Molec. Spectrosc. 19, 185-7
- (66.63a) R. A. McFarlane,
"Precision Spectroscopy of New Infrared Emission Systems of
Molecular Nitrogen,
IEEE J. Quant. Electronics QE-2, 229-32
- (66.64) w - a System. Laser Stimulated Transition,
R. A. MacFarlane,
Phys. Rev. 146, 37-9
- (66.64a) V. M. Kaslin and G. C. Petrash,
"Rotational Structure of Ultraviolet Generation of Molecular Nitrogen,"
JETP Letters 3, 55-57

- (66.65) J. W. Moskowitz, D. Neumann, and M. C. Harrison,
Molecules and the Solid State
Academic Press, Inc., New York
- (66.65a) K. C. Joshi,
"Relative Band Strengths and r-Centroids for the $B'^3\Sigma_u^- - Z^1\Sigma_g^+$
System of Nitrogen,"
Nature 212, 1459-60
- (67.66) Rydberg Series,
P. K. Carroll and K. Yoshino,
J. Chem. Phys. 47, 3073-4
- (67.67) a" - X Quadrupole Transition,
K. Dressler and B. L. Lutz,
Phys. Rev. Letters 19, 1219-21
- (67.68) B. K. Ching, G. R. Cook, and R. A. Becker,
"Oscillator Strengths of the a, w and C Bands of N₂,"
J. Quant. Spectrosc. Radiative Trans. 7, 323-30
- (67.68a) T. Kasuya and D. R. Lide, Jr.,
"Measurements on the Molecular Nitrogen Pulsed Laser,"
Appl. Optics 6, 66-80
- (68.69) N. A. Borisevich, M. V. Dubovik, and A. Ya. Smirnov,
Zhur. Priklad. Spectrosc. 9, 807-11
- (68.70) J. F. M. Aarts, F. J. DeHeer, and D. A. Vroom,
"Emission Cross Sections of the First Negative Band System of N₂
by Electron Impact,"
Physica 40, 197-206
- (68.71) P. N. Stanton,
"Electron Excitation of the First Positive Bands of N₂ and of the
First Negative and Meinel Bands of N₂⁺,"
Thesis, University of Oklahoma
- (68.72) S. N. Ghosh, Y. Sahai, and K. K. Bhutani,
"Spectra of N₂ Excited by Proton Bombardment,"
Indian J. Phys. 42, 146-7
- (68.73) H. L. Wu and W. Benesch,
"Evidence for the $^3\Delta_u \rightarrow B^3\Pi_g$ Transition in N₂,"
Phys. Rev. 172, 31-5
- (68.74) Yu. A. Plastinin,
"Optical Absorption Cross Sections of Two Atom Molecules,"
Fiz. Gazodin. Ioniz. Khim. Reag. Gazov. 89-125

- (68. 74a) J. H. Parks, D. R. Rao, and A. Jowan,
"A High Resolution Study of the $C^3\Pi_u - B^3\Pi_g$ (0, 0) Stimulated
Transitions in N_2 ,"
Appl. Phys. Letters 13, 142-4
- (68. 75) Vegard-Kaplan System,
C. Chandraiah and G. G. Shepherd,
Can. J. Phys. 46, 221-6
- (68. 76) Oscillator Strengths,
G. M. Lawrence, D. L. Mickey, and K. Dressler,
J. Chem. Phys. 48, 1989-94
- (68. 77) Spectra of Solid N_2 ,
J. Y. Roncin,
J. Molec. Spectrosc. 26, 105-10
- (68. 78) Raman Spectra,
J. J. Barrett and N. I. Adams III,
J. Opt. Soc. Am. 58, 311-9
- (68. 79) W - B System,
H. L. Wu and W. Benesch,
Phys. Rev. 172, 31-5
- (68. 80) A. N. Wright and C. A. Winkler,
Active Nitrogen
Academic Press, New York
- (69. 81) High Resolution Absorption Study in the Vacuum Ultraviolet,
P. K. Carroll and C. P. Collins,
Can. J. Phys. 47, 563-90
- (69. 82) Rydberg States,
K. Dressler,
Can. J. Phys. 47, 547-61
- (69. 83) Theory of Homogeneous Perturbation,
H. Lefebvre-Brion,
Can. J. Phys. 47, 541-6
- (69. 84) D. J. Burns, F. R. Simpson, and J. W. McConkey,
"Absolute Cross Sections for Electron Excitation of the Second
Positive Bands of Nitrogen,"
J. Phys. B (Atom. Molec. Phys.) 2, 52-64
- (69. 85) J. W. McConkey and F. R. Simpson,
"Electron Impact Excitation of the $B^3\Pi_g$ State of N_2 ,"
J. Phys. B (Atom. Molec. Phys.) 2, 923-9

- (69. 86) P. N. Stanton and R. M. St. John,
"Electron Excitation of the First Positive Bands of N₂ and of the
First Negative and Meinel Bands of N₂⁺,"
J. Opt. Soc. Am. 59, 252-60
- (69. 87) D. H. Stedman and D. W. Setser,
"Energy Pooling by Triplet Nitrogen (A³Σ_u⁺) Molecules,"
J. Chem. Phys. 50, 2256-8
- (69. 88) R. S. Freund,
"Molecular-Beam Measurements of the Emission Spectrum and
Radiative Lifetime of N₂ in the Metastable E³Σ_g⁺ State,"
J. Chem. Phys. 50, 3734-40
- (69. 89) M. R. Katti and H. D. Sharma,
"Evaluation of r-Centroids for the Band Systems of a Few Diatomic
Molecules Using the Hulburt-Hirschfelder Potential Function,"
Indian J. Pure Appl. Phys. 7, 282-3
- (69. 90) J. Geiger and B. Schröder,
"Intensity Perturbations Due to Configuration Interaction Observed
in the Electron Energy-Loss Spectrum of N₂,"
J. Chem. Phys. 50, 7-16
- (70. 91) M. J. Hubin-Franskin and J. E. Collin,
"Electron Impact Excitation by the SF₆ Scavenger Technique
I. Nitrogen,"
Int. J. Mass Spectrom. Ion Phys. 4, 451-63
- (70. 92) K. A. Saum and W. M. Benesch,
"Infrared Electronic Emission Spectrum of Nitrogen,"
Appl. Optics 9, 195-200
- (70. 93) A. W. Johnson and R. G. Fowler,
"Measured Lifetimes of Rotational and Vibrational Levels of
Electronic States of N₂,"
J. Chem. Phys. 53, 65-72
- (70. 94) K. A. Saum and W. M. Benesch,
W³Δ_u - X¹Σ_g⁺ System of N₂,"
Phys. Rev. A 2, 1655-9
- (70. 95) D. C. Cartwright,
"Total Cross Sections for the Excitation of the Triplet States in
Molecular Nitrogen,"
Phys. Rev. A 2, 1331-48

- (70. 96) H. H. Michels,
"Identification of Two Low-Lying Non-Rydberg States of the
Nitrogen Molecule,"
J. Chem. Phys. 53, 841-2
- (70 97) D. W. Setser, D. H. Stedman, and J. A. Coxon,
"Chemical Applications of Metastable Argon Atoms. IV. Excitation
and Relaxation of Triplet States of N₂,"
J. Chem. Phys. 53, 1004-20
- (70. 98) K. L. Wray, E. V. Feldman, and P. F. Lewis,
"Shock Tube Study of the Effect of Vibrational Energy of N₂ on the
Kinetics of the O + N₂ → NO + N Reaction,"
J. Chem. Phys. 53, 4131-6
- (70. 99) D. C. Jain,
"A Study of Some Potential Energy Functions for Diatomic Molecules,"
Int. J. Quantum Chem. 4, 579-85
- (70. 100) A. A. Griбанова, V. V. Kokhaenko, N. A. Prilezhaeva, and
L. A. Sigaenko,
"On the Question of the Intensity Distribution in the Rotational
Structure and Electronic-Vibrational Bands of Nitrogen,"
Izvest. Vyssh. Ucheb. Zaved. Fiz. 9, 17-21
- (71. 101) W. M. Benesch and K. A. Saum,
"The W³Δ_u State of Molecular Nitrogen,"
J. Phys. B (Atom. Molec. Phys.) 4, 732-8
- (71. 102) M. F. Golde and B. A. Thrush,
"Vacuum Ultraviolet Emission by Active Nitrogen,"
Chem. Phys. Letters 8, 375-7
- (71. 103) J. M. Calo and R. C. Axtmann,
"Vibrational Relaxation and Electronic Quenching of the C ³Π_u
(v' = 1) State of Nitrogen,"
J. Chem. Phys. 54, 1332-41
- (71. 104) T. T. Kassal and E. S. Fishburne,
"Energy Transfer Between N₂ and Electronically Excited Inert Gas
Atoms and Ions,"
J. Chem. Phys. 54, 1363-8
- (71. 105) W. E. Sharp,
"Rocket-Borne Spectroscopic Measurements in the Ultraviolet
Aurora: Nitrogen Vegard-Kaplan Bands,"
J. Geophys. Res. 76, 987-1005

- (72. 106) W. L. Borst,
"Excitation of Several Important Metastable States of N₂ by
Electron Impact,"
Phys. Rev. A 5, 648-56
- (72. 107) S. N. Ghosh and S. K. Gupta,
"Effect of Molecular Oxygen and Temperature on the N₂ First
Positive Bands in the Nitrogen Afterglow,"
Indian J. Phys. 46, 18-27
- (72. 108) J. H. Moore, Jr.,
"Electronic Excitation of N₂ and Dissociative Excitation of O₂ by
Proton Impact,"
J. Geophys. Res. 77, 5567-72
- (72. 109) N. Bjorna,
"Density-Distribution Analysis of a Constrained SCF-LCAO-MO
Wave Function for N₂,"
Phys. Norvegica 6, 81-5
- (72. 110) J. W. Dreyer and D. Perner,
"The Deactivation of N₂B³Π_g, v=0-2 and N₂a¹Σ_u⁻, v=0 by
Nitrogen,"
Chem. Phys. Letters 16, 169-73
- (72. 111) R. J. McNeal, M. E. Whitson, Jr., and G. R. Cook,
"Quenching of Vibrationally Excited N₂ by Atomic Oxygen,"
Chem. Phys. Letters 16, 507-10
- (72. 112) D. G. Truhlar,
"Test of Massey's Method for Calculating the Static Potential for
Electron Scattering by N₂,"
Chem. Phys. Letters 15, 486-9
- (72. 113) D. G. Truhlar, F. A. Van-Catledge, and T. H. Dunning,
"Ab Initio and Semiempirical Calculations of the Static Potential
for Electron Scattering Off the Nitrogen Molecule,"
J. Chem. Phys. 57, 4788-99
- (72. 114) S. J. Young and K. P. Horn,
"Measurements of Temperatures of Vibrationally Excited N₂,"
J. Chem. Phys. 57, 4835-46
- (72. 115) R. J. McNeal, M. E. Whitson, Jr., and G. R. Cook,
"Photoionization of Vibrationally Excited N₂. II. Quenching by
CO₂ and N₂O,"
J. Chem. Phys. 57, 4752-8

- (72. 116) L. S. Polak, D. I. Slovetskii, and A. S. Sokolov,
 "Predissociation and Quenching Probabilities for the Vibrational
 Levels of the B³Π_g State of Molecular Nitrogen,"
Opt. Spectrosc. 32, 247-51
- (72. 117) A. A. Konkov and A. V. Vorontsov,
 "Experimental Study of Nitrogen Infrared Radiation,"
Opt. Spectrosc. 32, 348-50
- (72. 118) J. B. Tellinghuisen, C. A. Winkler, C. G. Freeman, M. J. McEwan,
 and L. F. Phillips,
 Quenching Rates for N₂⁺, N₂O⁺, and CO₂⁺ Emission Bands Excited
 by 58.4 nm Irradiation of N₂, N₂O, and CO₂,"
J. Chem. Soc. Faraday Trans. II 68, 833-8
- (72. 119) P. G. Burke and N. Chandra,
 "Electron-Molecule Interactions III. A Pseudo-Potential Method
 for e⁻-N₂ Scattering,"
J. Phys. B (Atom. Molec. Phys.) 5, 1696-1711
- (72. 120) R. G. Gann, F. Kaufman, and M. A. Biondi,
 "Interferometric Study of the Chemiluminescent Excitation of
 Sodium by Active Nitrogen,"
Chem. Phys. Letters 16, 380-4
- (72. 121) G. C. Berend, R. L. Thommarson, and S. W. Benson,
 "Vibration-Vibration Energy Exchange in N₂ With O₂ and HCl
 Collision Partners,"
J. Chem. Phys. 57, 3601-4
- (72. 122) D. G. Truhlar,
 "Vibrational Matrix Elements of the Quadrupole Moment Functions
 of H₂, N₂ and CO,"
Int. J. Quant. Chem. 6, 975-88
- (72. 123) D. Spence, J. L. Mauer, and G. J. Schulz,
 "Measurement of Total Inelastic Cross Sections for Electron
 Impact in N₂ and CO₂,"
J. Chem. Phys. 57, 5516-21
- (72. 124) N. Bjorna,
 "Methods for Solving Constrained SCF-LCAO-MO Equations.
 Application to a Calculation on N₂,"
Molec. Phys. 24, 1-10

- (72. 125) E. Kisker,
"Optical Measurement of Electron-Impact Excitation of Xenon and Molecular Nitrogen in the Threshold Region With High Energy Resolution,"
Z. Physik 257, 51-61
- (72. 126) R. F. Holland and W. B. Maier II,
"Emission From Long-Lived States of N₂⁺. A New Interpretation of N₂⁺+N₂→N₃⁺+N,"
J. Chem. Phys. 57, 4497-8
- (72. 127) P. C. Cosby and T. F. Moran,
"Product Internal State Distributions From Interactions of Meta-stable Ar With N₂,"
J. Chem. Phys. 57, 4111-5
- (72. 128) W. Von Niessen,
"Density Localization of Atomic and Molecular Orbitals,"
Theoret. Chim. Acta 27, 9-23
- (72. 129) R. Simonaitis and J. Heicklen,
"The H_g(¹P₁) Sensitized Photolysis of N₂ and CO,"
J. Photochem. 1, 181-97
- (72. 130) R. Carbonneau and P. Marmet,
"Autoionizing Levels of N₂ Converging to the A²Π_u and B²Σ_u⁺ Limits,"
Int. J. Mass Spectrom. Ion Phys. 10, 143-55
- (72. 131) G. Hartmann,
"Relative Populations of the C³Π_u and B³Σ_u⁺ States of Nitrogen Created by the Passing of a Predisruptive Discharge Through Flames,"
C. R. Acad. Sci. B 275, 311-4
- (72. 132) M. Leoni and K. Dressler,
"Deperturbation of the Worley-Jenkins Rydberg Series of N₂,"
Helv. Phys. Acta 45, 959-961
- (72. 133) S. Chung and C. C. Lin,
"Excitation of the Electronic States of the Nitrogen Molecule by Electron Impact,"
Phys. Rev. A 6, 988-1002
- (72. 134) D. C. Cartwright, W. Williams, and S. Trajmar,
"The IR Emission Spectrum of N₂ Excited Under Auroral Conditions,"
Ann. Geophys. 28, 403-7

- (72. 135) N. P. Danilevskii, L. I. Popova, A. G. Koval, N. I. Fedorova, V. T. Koppe, and Ya. M. Fogel,
"The Infrared Spectrum of Nitrogen Excited by Fast Electrons,"
Ann. Geophys. 28, 409-14
- (72. 136) A. Sharma and J. C. Joshi,
"The Mechanism of Vacuum Ultraviolet Emission From the Lewis-Rayleigh Nitrogen Afterglow,"
J. Quant. Spectrosc. Radiative Trans. 12, 1641-6
- (72. 137) B. A. Thrush and A. H. Wild,
"Excitation of Species in Active Nitrogen, Part 1. - Mercury Hg(6^3P_1),"
J. Chem. Soc. Faraday Trans. II 68, 2023-30
- (73. 138) R. S. Hickman and L. Liang,
"Comment on 'Rotational Temperature Measurement in Nitrogen',"
Rev. Sci. Instrum. 44, 246
- (73. 139) V. I. Kleimenov, Yu. V. Chizhov, and F. I. Vilesov,
"Applicability of the Franck-Condon Principle to the Autoionization of the N₂ Molecule,"
Opt. Spectrosc. 34, 590
- (73. 140) P. Millet, Y. Salamero, H. Brunet, J. Galy, and D. Blanc,
"De-excitation of N₂ ($C^3\Pi_u$; $v' = 0$ and 1) Levels in Mixtures of Oxygen and Nitrogen,"
J. Chem. Phys. 58, 5839-41
- (73. 141) S. A. Lawton and F. M. J. Pichanick,
"Resonances in the Metastable Excitation of Molecular Nitrogen,"
Phys. Rev. A 7, 1004-7
- (73. 142) A. I. Lyutui and L. D. Meinikov,
"Excitation Temperature for Active Nitrogen,"
Opt. Spectrosc. 34, 385-6
- (73. 143) M. Outred and M. E. Pillow,
"Some Observations on the Decay of the Lewis-Rayleigh Afterglow in a Nitrogen-Oxygen Mixture,"
J. Phys. B (Atom. Molec. Phys.) 6, 2701-6
- (73. 144) L. S. Polak and D. I. Slovetskii,
"Electron-Impact Vibrational Excitation Cross Sections for Molecular Nitrogen,"
High Temp. 10, 575-6

- (73. 155) W. L. Borst and S. L. Chang,
"Excitation of Metastable N₂(A $^3\Sigma_u^+$) Vibrational Levels by
Electron Impact,"
J. Chem. Phys. 59, 5830-6
- (73. 156) A. Crowe and J. W. McConkey,
"Dissociative Ionization by Electron Impact II. N⁺ and N⁺⁺
From N₂,"
J. Phys. B (Atom. Molec. Phys.) 6, 2108-17
- (73. 157) J. M. Hoffman, G. J. Lockwood, and G. H. Miller,
"Emission Cross Sections for the N₂ Second Positive (0,0)
Transition for H, H⁺, He, and He⁺ Impact,"
Phys. Rev. A 7, 118-25
- (73. 158) A. Chutjian, D. C. Cartwright, and S. Trajmar,
"Excitation of the W $^3\Delta_u$, w $^1\Delta_u$, B $^3\Sigma_u^-$, and a $^1\Sigma_u^-$ States of N₂ by
Electron Impact,"
Phys. Rev. Letters 30, 195-8
- (73. 159) L. Klynning,
"On the 6895.5Å and 8937.0Å Bands of N₂,"
Spectrosc. Letters 6, 291-2
- (73. 160) H. A. Hyatt, J. M. Cherlow, W. R. Fenner, and S. P. S. Porto,
"Cross Section for the Raman Effect in Molecular Nitrogen Gas,"
J. Opt. Soc. Am. 63, 1604-6
- (73. 161) K. C. Smyth, J. A. Schiavone, and R. S. Freund,
"Dissociative Excitation of N₂ by Electron Impact: Translational
Spectroscopy of Long-Lived High-Rydberg Fragment Atoms,"
J. Chem. Phys. 59, 5225-41
- (73. 162) A. I. Dashchenko, I. P. Zapesochnyi, and A. I. Imre,
"Excitation Cross Sections of Bands of the First Negative System
of Nitrogen in Electron-Ion Collisions,"
Opt. Spectrosc. 35, 970-2
- (73. 163) B. W. Woodward, V. J. Ehlers, and W. C. Lineberger,
"A Reliable, Repetitively Pulsed, High-Power Nitrogen Laser,"
Rev. Sci. Instrum. 44, 882-7
- (73. 164) L. Y. Nelson, G. J. Mullaney, and S. R. Byron,
"Superfluorescence in N₂ and H₂ Electron-Beam-Stabilized
Discharges,"
Appl. Phys. Letters 22, 79-80

- (73. 165) I. Nagata and Y. Kimura,
"A Compact High-Power Nitrogen Laser,"
J. Phys. E (Sci. Instrum.) 6, 1103-5
- (73. 166) G. Joyez, R. I. Hall, J. Reinhardt, and J. Mazeau,
"Low Energy Electron Spectroscopy of N₂ in the 11.8-13.8 eV
Energy Range,"
J. Electron. Spectrosc. Rel. Phenom. 2, 183-90
- (73. 167) R. Covey, K. A. Saum, and W. Benesch,
"Transition Probabilities for the W³Δ_u - B³Π_g System of Molecular
Nitrogen,"
J. Opt. Soc. Am. 63, 592-6
- (73. 168) A. A. Tagliaferri, M. Gallardo, C. A. Massone, and
M. Garavaglia,
"UV Stimulated Emission From N₂ and NO,"
Phys. Letters 45A, 211-2
- (73. 169) G. N. Hays and H. J. Oskam,
"Population of N₂(B³Π_g) by N₂(A ³Σ_u⁺) During the Nitrogen
Afterglow,"
J. Chem. Phys. 59, 1507-16
- (73. 170) P. J. Hicks, J. Comer, and F. H. Read,
"Autoionizing Transitions in N₂ and H₂ Produced by Electron
Impact,"
J. Phys. B (Atom. Molec. Phys.) 6, L65-L69
- (73. 171) W. E. Jones and M. Rujimethabhas,
"Reaction of Active Nitrogen With Tetrachloroethylene,"
Can. J. Chem. 51, 3680-3
- (73. 172) J. Rose, T. Shibuya, and V. McKoy,
"Application of the Equations-of-Motion Method to the Excited
States of N₂, CO, and C₂H₄,"
J. Chem. Phys. 58, 74-83
- (73. 173) L. S. Cederbaum, G. Hohlneicher, and W. Von Niessen,
"On the Breakdown of the Koopmans' Theorem for Nitrogen,"
Chem. Phys. Letters 18, 503-8
- (73. 174) V. I. Egorov, Yu. M. Gershenzon, V. B. Rosenshtein, and
S. Ya. Umanskii,
"On the Mechanism of Heterogeneous Relaxation of Vibrationally
Excited Nitrogen Molecules,"
Chem. Phys. Letters 20, 77-80

- (73. 145) L. Veseth,
 "On the Calculation of Molecular Parameters for Triplet States
 in Diatomic Molecules. The $G^3\Delta_g$ and $H^3\Phi_u$ States of N₂,"
Molec. Phys. 26, 101-7
- (73. 146) W. S. Watson, J. Lang, and D. T. Stewart,
 "Photoabsorption Coefficients of Molecular Nitrogen in the
 300-700 Å Region,"
J. Phys. B (Atom. Molec. Phys.) 6, L148-L151
- (73. 147) J. S. Briggs and M. R. Hayns,
 "Molecular Orbital Calculations for Close Atomic Collisions:
 The N₂ System,"
J. Phys. B (Atom. Molec. Phys.) 6, 514-20
- (73. 148) J. Comer and M. Harrison,
 "Observation of the Effects of Rotational Transitions in the
 Resonant Scattering of Electrons From N₂,"
J. Phys. B (Atom. Molec. Phys.) 6, L70-L72
- (73. 149) R. W. Dreyfus and R. T. Hodgson,
 "Relativistic Electron-Beam Pumped uv Gas Lasers,"
J. Vac. Sci. Tech. 10, 1033-6
- (73. 150) J. W. Dreyer and D. Perner,
 "Deactivation of N₂ ($A^3\Sigma_u^+$, $v = 0-7$) by Ground State Nitrogen,
 Ethane, and Ethylene Measured by Kinetic Absorption Spectroscopy,"
J. Chem. Phys. 58, 1195-1201
- (73. 151) G. R. Cook, M. Ogawa, and R. W. Carlson,
 "Photodissociation Continuums of N₂ and O₂,"
J. Geophys. Res. 78, 1663-7
- (73. 152) L. C. Lee, R. W. Carlson, D. L. Judge, and M. Ogawa,
 "The Absorption Cross Sections of N₂, O₂, CO, NO, CO₂, N₂O,
 CH₄, C₂H₄, C₂H₆ and C₄H₁₀ From 180 to 700 Å,"
J. Quant. Spectrosc. Radiative Trans. 13, 1023-31
- (73. 153) D. DeSantis, A. Lurio, T. A. Miller, and R. S. Freund,
 "Radio-Frequency Spectrum of Metastable N₂($A^3\Sigma_u^+$). II. Fine
 Structure, Magnetic Hyperfine Structure, and Electric Quadrupole
 Constants in the Lowest 13 Vibrational Levels,"
J. Chem. Phys. 58, 4625-65
- (73. 154) G. N. Hays and H. J. Oskam,
 "Reaction Rate Constant for $2N_2(A^3\Sigma_u^+) \rightarrow N_2(C^3\Pi_u) + N_2(X^1\Sigma_g^+, v' > 0)$,"
J. Chem. Phys. 59, 6088-91

- (73. 175) L. Kurzweg, G. T. Egbert, and D. J. Burns,
"Contribution of the Metastable $E^3\Sigma_g^+$ State to the Population of
the $C^3\Pi_u$ State of N_2 Following Electron-Impact Excitation,"
Phys. Rev. A 7, 1966-71
- (73. 176) O. V. Ravodina, T. N. Popova, A. A. Eliseev, and S. S. Smolyakov,
"Excitation of the $B^3\Pi_g$ State of Molecular Nitrogen in a Glow
Discharge,"
Opt. Spectrosc. 34, 243-5
- (73. 177) L. W. Dotchin and E. L. Chupp,
"Radiative Lifetimes and Pressure Dependence of the Relaxation
Rates of Some Vibronic Levels in N_2^+ , N_2 , CO^+ , and CO ,"
J. Chem. Phys. 59, 3960-7
- (73. 178) M. Czajkowski, L. Krause, and G. M. Skardis,
"Quenching of Mercury-Sensitized Fluorescence in Sodium
Induced in Collisions With N_2 Molecules,"
Can. J. Phys. 51, 1582-9
- (73. 179) M. J. W. Boness and G. J. Schulz,
"Excitation of High Vibrational States of N_2 and CO via Shape
Resonances,"
Phys. Rev. A 8, 2883-6
- (73. 180) V. A. Kosinov and P. A. Skovorodko,
"Calculation of the Franck-Condon Factors for the Processes
Involved in the Excitation of the Molecular Bands of the First
Negative System of Nitrogen and Carbon Monoxide,"
Opt. Spectrosc. 34, 344
- (73. 181) E. A. Andreev,
"Energy Transfer in N_2 -Alkali Collisions,"
Chem. Phys. Letters 23, 516-7
- (73. 182) L. Kurzweg, G. T. Egbert, and D. J. Burns,
"Lifetime of the $D^3\Sigma_u^+$ State of N_2 ,"
J. Chem. Phys. 59, 2641-45
- (73. 183) A. Corney,
"Measurements of Transition Probabilities of Forbidden Lines of
Neutral Atoms and Molecules,"
Nuc. Instrum. Methods 110, 151-66
- (73. 184) A. Pochat, M. Doritch, and J. Pereese,
"Measurement of the Absolute Lifetimes of Helium, Neon,
Molecular Nitrogen and Carbon Monoxide,"
J. Chim. Phys. 70, 936-40

- (73. 185) F. P. Billingsley II,
"Quadrupole Moment of CO, N₂ and NO⁺,"
J. Chem. Phys. 60, 2767-72
- (74. 186) J. M. Hoffman, G. J. Lockwood, and G. H. Miller,
"Emission Cross Sections for N₂⁺(3914 Å) for F⁺, Ne⁺, and Na⁺
Ions Incident on N₂ Gas,"
Phys. Rev. A 9, 187-91
- (74. 187) V. N. Lisitin, P. L. Chapovski, and A. A. Chernenko,
"Monochromatization of Emission Frequency of the Infrared
Nitrogen Laser,"
Kvant. Elekt. 1, 341-5
- (74. 188) P. K. Carroll and A. P. Doheny,
"The Herman-Kaplan System of N₂: High Resolution Studies,"
J. Molec. Spectrosc. 50, 257-65
- (74. 189) S. K. Searles and G. A. Hart,
"Laser Emission at 3577 and 3805 Å in Electron-Beam-Pumped
Ar-N₂ Mixtures,"
Appl. Phys. Letters 25, 79-82
- (74. 190) E. R. Ault, M. L. Bhaumik, and N. T. Olson,
"High-Power Ar-N₂ Transfer Laser at 3577 Å,"
J. Quant. Elect. QE-10, 624-6
- (74. 191) B. Godard,
"A Simple High-Power Large-Efficiency N₂ Ultraviolet Laser,"
J. Quant. Elect. QE-10, 147-53
- (74. 192) R. A. Young,
"New Theory of Active Nitrogen,"
J. Chem. Phys. 60, 5050-3
- (74. 193) D. A. McArthur and J. W. Poukey,
"Theory of Plasma Electron Contribution to the Electron-Beam-
Excited Nitrogen Laser,"
Phys. Rev. Letters 32, 89-92
- (74. 194) W. Brennen, R. V. Gutowski, and E. C. Shane,
"Vibrational Distributions of N₂(A³Σ_u⁺) in the Nitrogen Afterflow,"
Chem. Phys. Letters 27, 138-140
- (74. 195) H. Fischer, R. Girnus, and F. Rühl,
"Low Threshold Coaxial N₂ Laser With a Resonator,"
Appl. Optics 13, 1759-60

- (74. 196) M. Imami and W. L. Borst,
"Electron Excitation of the (0,0) Second Positive Band of Nitrogen
From Threshold to 1000 eV,"
J. Chem. Phys. 61, 1115-7
- (74. 197) R. T. Brown and D. C. Smith,
"Optically Pumped Electric-Discharge uv Laser,"
Appl. Phys. Letters 24, 236-8
- (74. 198) D. H. Winicur and J. L. Fraites,
"Electronic-Energy Exchange Cross Sections for Ar*(³P) and N₂
(X¹Σ_g⁺),"
J. Chem. Phys. 71, 1548-53
- (74. 199) H. E. B. Andersson and R. C. Tobin,
"Electrical Breakdown and Pumping in an Axial-Field Nitrogen
Laser,"
Physica Scripta 9, 7-14
- (74. 200) G. C. Lie and E. Clementi,
"Study of the Electronic Structure of Molecules. XXII. Correla-
tion Energy Corrections as a Function of the Hartree-Fock Type
Density and its Application to the Homonuclear Diatomic Molecules
of the Second Row Atoms,"
J. Chem. Phys. 60, 1288-96
- (74. 201) K. J. Miller and A. E. S. Green,
"Energy Levels and Potential Energy Curves for H₂, N₂, and O₂
With an Independent Particle Model,"
J. Chem. Phys. 60, 2617-26
- (74. 202) G. C. Baldwin,
"Nitrogen Total Cross Section for Electrons Below 2.0 eV,"
Phys. Rev. A 9, 1225-9
- (74. 203) T. G. Slinger and G. Black,
"Electronic-to-Vibrational Energy Transfer Efficiency in the
O(¹D)-N₂ and O(¹D)-CO Systems,"
J. Chem. Phys. 60, 468-77
- (74. 204) S. N. Suchard, L. Galvan, and D. G. Sutton,
"Quasi-CW Laser Emission From the Second Positive Band of
Nitrogen,"
First Summer Coll. Elect. Transition Lasers (Unpublished)
- (74. 205) S. K. Searles,
"Superfluorescent Laser Emission From Electron-Beam-Pumped
Ar-N₂ Mixtures,"
Appl. Phys. Letters 25, 735-7

- (74.206) J. I. Levatter and S. C. Lin,
"High-Power Generation From a Parallel-Plates-Driven Pulsed Nitrogen Laser,"
Appl. Phys. Letters 25, 703-5
- (74.207) T. D. Nguyen, N. Sadeghi, and J. C. Pebay-Peyroula,
"Energy Transfer Reaction Between Metastable Xenon Atoms and Nitrogen Molecules: Excitation of the N₂(B ³Π_g, v' ≤ 5) States in the Afterglow,"
Chem. Phys. Letters 29, 242-6
- (74.208) V. N. Ishchenko, V. N. Lisitsyn, A. M. Razhev, and V. N. Starinskii,
"Superradiance on the 2⁺ and 1⁻ Bands of Nitrogen in a Discharge at Pressures Above 10 atm,"
JETP Letters 19, 233-4
- (74.209) V. Hasson, D. Preussler, J. Klimek, and H. M. von Bergmann,
"Transverse Double-Discharge High-Pressure Glow Excitation of uv Lasing Action in Molecular Nitrogen,"
Appl. Phys. Letters 25, 654-6
- (74.210) F. Albugues, A. Birot, D. Blanc, H. Brunet, J. Galy, and P. Millet,
"Destruction of the Levels C ³Π_u (v' = 0, v' = 1) of Nitrogen by O₂, CO₂, CH₄, and H₂O,"
J. Chem. Phys. 61, 2695-9
- (74.211) J. H. Birely,
"Formation of N₂⁺ B ²Σ_u⁺ and N₂ C ³Π_u in Collisions of H⁺ and H With N₂,"
Phys. Rev. A 10, 550-62
- (74.212) P. K. Carroll and A. P. Doheny,
"The Herman-Kaplan System of N₂: High Resolution Studies,"
J. Molec. Spectrosc. 50, 257-65
- (74.213) D. C. Cartwright and T. H. Dunning, Jr.,
"Vibrational Matrix Elements of the Quadrupole Moment of N₂ (x ¹Σ_g⁺),"
J. Phys. B (Atom. Molec. Phys.) 7, 1776-81
- (74.214) J. W. Dreyer, D. Perner, and C. R. Roy,
"Rate Constants for the Quenching of N₂(A ³Σ_u⁺, v_A = 0-8) by CO, CO₂, NH₃, NO, and O₂,"
J. Chem. Phys. 61, 3164-9

- (74.215) K. J. Rajan,
 "The 1-0 Band of the $b^1\Pi_u - a^1\Pi_g$ Transition and the 1-10 and 2-12 Bands of the Fifth Positive System of N_2 . Rotational Analyses,"
Proc. Roy. Irish Acad. A 74, 17-23
- (75.216) C. S. Willett and D. M. Litynski,
 "Power Increase of N_2 uv and ir Lasers by Addition of SF_6 ,"
Appl. Phys. Letters 26, 118-21
- (n.p.217) S. N. Suchard, R. F. Heidner III, and D. G. Sutton,
 Behavior of the First and Second Positive Emission in the N_2/SF_6 Laser,"
 (to be published IEEE J. Quant. Electron Nov. 1975)
- (n.p.218) S. N. Suchard and D. G. Sutton,
 Private Communication
- (66.L1) M. Jeunehomme
 "Transition Moment of the First Positive Band System of Nitrogen,"
J. Chem. Phys. 45, 1805-11
- (69.L2) D. E. Shemansky, N. P. Carleton
 "Lifetime of the N_2 Vegard-Kaplan System,"
J. Chem. Phys. 51, 682-8
- (69.L3) D. E. Shemansky
 " N_2 Vegard-Kaplan System in Absorption,"
J. Chem. Phys. 51, 689-700

Na₂

Na₂

Methods of Production and Experimental Technique

Absorption.

Emission from a discharge in Na₂ vapor, heat pipe.

Fluorescence.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$A^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$	Absorption, discharge, fluorescence	8000-6000	R			(70.44, 33.20, 29.13)
	II	$B^1\Pi_u \rightarrow X^1\Sigma_g^+$	Absorption, discharge, fluorescence	5040-4560	R			(69.41, 32.17, 28.10)
	III	$C^1\Pi_u \rightarrow X^1\Sigma_g^+$	Absorption, discharge	3600-3200	R	3338.8(5,0) 3326.3(6,0)		(50.34, 49.33)
	IV	$D^1\Pi_u \rightarrow X^1\Sigma_g^+$	Absorption	3325-3030	R			(50.34)
	V	$E \rightarrow ?$	Absorption, discharge	3120-2880	R	2945.5(7,0)		(47.31)
	VI	$? \rightarrow ?$	Absorption, discharge	3050-2500	R	2750, 2735		(47.31)

Molecule Na₂

I. $A^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$ System

Most intense band heads in absorption, λ (33.20, 29.13):

(v', v'')	(4, 2)	(4, 1)	(5, 1)	(6, 0)	(7, 0)	(8, 0)	(9, 0)
λ	6751.2	6679.7	6561.5	6513.2	6465.8	6418.4	6374.2

II. $B^1\Pi_u \leftarrow X^1\Sigma_g^+$ System

Most intense band heads in absorption, λ (32.17, 28.10):

(v', v'')	(0, 3)	(0, 2)	(0, 1)	(1, 1)	(0, 0)	(1, 0)	(2, 0)	(3, 0)
λ	5040.4	5001.4	4962.8	4932.6	4924.2	4894.5	4865.5	4837.2

III. $C^1\Pi_u \leftarrow X^1\Sigma_g^+$ System

Most intense band heads, λ (absorption intensity, emission intensity) (50.34, 49.3):

(v', v'')	(5, 1)	(4, 0)	(5, 0)	(6, 0)	(7, 0)	(9, 0)	(10, 0)
λ	3356.5	3351.5	3338.8	3326.3	3314.0	3290.0	3278.4
Absorption intensity	8	7	10	10	10	9	8
Emission intensity	4	4	5	4	4	4	4

IV. $D^1\Pi_u \leftarrow X^1\Sigma_g^+$ System

Most intense band heads, λ (Intensity) (50.34):

(v', v'')	(1, 2)	(3, 3)	(2, 2)	(1, 1)	(0, 0)	(2, 1)	(1, 0)	(2, 0)
λ	3151.6	3145.2	3140.0	3135.7	3131.2	3125.1	3120.5	3109.5
(Intensity)	2	2	2	2	2	2	2	2

V. E ≈ ? System

Most intense band heads, λ (absorption intensity, emission intensity) (47.31):

λ	2983.1	2959.6	2945.5	2936.2	2932.5	2928.6	2927.6
Absorption intensity	6	6	10	8	6	6	8
Emission intensity	0	0	0	4	2	2	4

VI. 3050-2500Å Bands

Possibly four fragmentary systems (4-7), preliminary vibrational analysis, λ (Intensity) (47.31):

(v', v'')	(0, 3)	(1, 3)	(0, 1)	(2, 1)	(0, 0)	(1, 0)	(2, 0)	(8, 0)	(0, 6)
λ	2986.4	2977.0	2958.6	2948.2	2944.0	2935.6	2970.6	2750.0	2735.0
Intensity	6	5	5	6	5	8	5	5	5
System	4	4	4	4	4	4	4	5	6

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e \omega_e$	B_e	$\alpha_e \times 10^4$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$D^1\Pi_u$	33486.9	111.93	0.573	0.1152	11.0				(60.35)
$C^1\Pi_u$	29384.8	119.53	0.782	0.1185	9.6				(60.35, 32.17)
$B^1\Pi_u$	20319.596	124.065	0.6863	0.125829	8.6754	0.3614	3.41398	(a)	(69.41, 32.17)
$A^1\Sigma_u^+$	14680.4	117.6	0.38	0.1107	5.4		3.64		(29.13)
$b\Pi(0_u^+)$ (b)	<14680.4	~ 145		~ 0.14					(33.21)
$X^1\Sigma_g^+$	0	159.126	0.7262	0.154853	8.5637	0.6552	3.07745	(c)	(69.41, 33.20)

(a) $y_e \omega_e = -5.441 \times 10^{-3}$, $z_e \omega_e = -1.15 \times 10^{-4}$, $\gamma_e = -1.535 \times 10^{-5}$; (b) calculated by deperturbation analysis of $A^1\Sigma_u^+$; (c) $y_e \omega_e = -9.145 \times 10^{-3}$, $z_e \omega_e = -5.02 \times 10^{-5}$, $\gamma_e = -7.646 \times 10^{-6}$

Dissociation energy = 0.75 ± 0.03 eV, 17.3 kcal/mole, 6049 cm^{-1} .

Perturbations and General Information

Gyromagnetic ratio (g_j) = 0.03892 nuclear magnetons (64.36).

$A^1\Sigma_u^+$ state is perturbed by the $b\Pi(0_u^+)$ state (33.21).

Radiative lifetimes:

$$A^1\Sigma_u^+, \tau_r = 10^{-7} - 10^{-6} \text{ sec (70.44)}$$

$$B^1\Pi_u, \tau_r = 6.41 \text{ nsec (69.43)}$$

Average polarizability (736°K) = $30 \times 10^{-24} \text{ cm}^3$ (74.55).

Transition moment for $B^1\Pi_u \rightarrow X^1\Sigma_g^+$ system (74.56):

$$D = 6.8 + 0.5r \quad 2.6\text{\AA} \leq r \leq 5.0\text{\AA}$$

Potential energy curves - RKR potential (69.40):

	State	v	E(v)cm ⁻¹	r _{min} (Å)	r _{max} (Å)
T _e = 0.0	X ¹ Σ _g ⁺	0	79.4	2.9481	3.2200
		1	237.2	2.8593	3.3320
		2	393.5	2.8014	3.4141
		3	548.2	2.7563	3.4841
		4	701.6	2.7187	3.5475
		5	853.4	2.6864	3.6065
		6	1003.6	2.6581	3.6624
		7	1152.3	2.6327	3.7163
		8	1299.3	2.6099	3.7686
		9	1444.9	2.5893	3.8196
		10	1588.8	2.5705	3.8699
		11	1731.0	2.5533	2.9195
		12	1871.7	2.5375	3.9687
		13	2010.7	2.5231	4.0176
		14	2148.0	2.5100	4.0665
		15	2283.6	2.4979	4.1153

	State	v	E(v)cm ⁻¹	r _{min} (Å)	r _{max} (Å)
T _e = 14680.4 cm ⁻¹	A ¹ Σ _u ⁺	0	58.7	3.4875	3.8037
		1	175.5	3.3839	3.9330
		2	291.6	3.3159	4.0268
		3	406.9	3.2626	4.1060
		4	521.5	3.2179	4.1769
		5	635.3	3.1789	4.2421
		6	748.3	3.1442	4.3032
		7	860.6	3.1128	4.3612
		8	972.1	3.0839	4.4168
		9	1082.9	3.0573	4.4703
		10	1192.9	3.0324	4.5222
		11	1302.1	3.0091	4.5728
		12	1410.6	2.9871	4.6221
		13	1518.3	2.9663	4.6704
		14	1625.3	2.9466	4.7178
		15	1731.5	2.9278	4.7645
T _e = 20319.596	B ¹ Π _u	0	61.7	3.2663	3.5747
		1	184.2	3.1678	3.7044
		2	305.4	3.1038	3.7998
		3	425.1	3.0539	3.8814
		4	543.4	3.0122	3.9553
		5	660.2	2.9759	4.0242
		6	775.4	2.9435	4.0895
		7	889.0	2.9141	4.1523
		8	1000.9	2.8870	4.2132
		9	1111.1	2.8618	4.2727
		10	1219.5	2.8381	4.3313
		11	1326.0	2.8157	4.3892
		12	1430.6	2.7943	4.4467
		13	1533.2	2.7737	5.5039
		14	1633.9	2.7539	4.5612
		15	1732.4	2.7347	4.6186

Na₂

Franck-Condon factors - RKR potential (69.41):

$B^1\Pi_u - X^1\Sigma_g^+$

v', v''	0	1	2	3	4	5	6	7	8
0	6.55-1	1.61-1	2.13-1	2.00-1	1.51-1	9.77-2	5.61-2	2.94-2	1.44-2
1	1.93-1	1.92-1	5.53-2	2.47-4	4.52-2	1.03-1	1.23-1	1.07-1	7.68-2
2	2.69-1	4.05-2	3.19-2	1.15-1	7.40-2	8.32-3	9.19-3	5.28-2	8.78-2
3	2.35-1	1.67-2	1.30-1	2.68-2	1.69-2	8.17-2	6.84-2	1.56-2	1.46-3
4	1.43-1	1.36-1	4.39-2	3.84-2	9.15-2	1.41-2	1.53-2	6.60-2	5.99-2
5	6.44-2	1.96-1	9.62-3	1.08-1	2.86-3	5.45-2	6.53-2	5.72-3	1.66-2
6	2.22-2	1.49-1	1.16-1	2.24-2	6.54-2	5.29-2	3.20-3	6.06-2	4.46-2
7	5.95-3	7.41-2	1.77-1	2.28-2	8.28-2	6.65-3	7.60-2	1.46-2	1.68-2
8	1.26-3	2.63-2	1.33-1	1.31-1	2.55-3	8.92-3	9.94-3	4.16-2	5.20-2

Franck-Condon factor followed by a factor of ten

BIBLIOGRAPHY

- (09. 1) A, B \rightleftharpoons X Systems,
R. W. Wood and F. E. Hackett,
Astrophys. J. 30, 339-72
- (11. 2) A, B \rightleftharpoons X Systems,
R. W. Wood and R. G. Galt,
Astrophys. J. 33, 72-80
- (24. 3) B \rightleftharpoons X System, Incorrect Vibrational Analysis,
H. G. Smith,
Proc Roy. Soc. A 106, 400-15
- (27. 4) A \rightleftharpoons X System, Vibrational and Rotational Analysis, B \rightleftharpoons X System,
Incorrect Rotational Analysis,
W. R. Fredrickson and W. W. Watson,
Phys. Rev. 30, 429-38
- (27. 5) B \rightleftharpoons X System,
F. W. Loomis,
Phys. Rev. 29, 607
- (27. 6) A \rightleftharpoons X System, Excitation Mechanism,
H. Schüler,
Z. Physik 43, 474-9
- (28. 7) B \rightleftharpoons X System,
F. W. Loomis,
Phys. Rev. 31, 323-32
- (28. 8) B \rightleftharpoons X System,
F. W. Loomis,
Phys. Rev. 31, 705
- (28. 9) A \rightleftharpoons X System,
F. W. Loomis and S. W. Nile, Jr.,
Phys. Rev. 32, 873-9
- (28. 10) B \rightleftharpoons X System, Vibrational Analysis,
F. W. Loomis and R. W. Wood,
Phys. Rev. 32, 223-36
- (28. 11) B \rightleftharpoons X System,
D. S. Villars,
Proc. Nat. Acad. Sci. 14, 508-11

- (28. 12) Ultraviolet Systems,
J. M. Walter and S. Barratt,
Proc. Roy. Soc. A 119, 257-75
- (29. 13) A \approx X System, Vibrational and Rotational Analysis. B \approx System,
Incorrect Rotational Analysis,
W. R. Fredrickson,
Phys. Rev. 34, 207-12
- (30. 14) Ultraviolet Systems, Incorrect Analysis,
W. Weizel and M. Kulp,
Ann. Phys. 4, 971-84
- (30. 15) E. Hutchisson,
Phys. Rev. 36, 410-20
- (32. 16) A \rightarrow X System,
Y. Uchida,
Japan J. Phys. 8, 25-50
- (32. 17) B \approx X System, Vibrational Analysis,
F. W. Loomis and R. E. Nussbaum,
Phys. Rev. 40, 380-6
- (32. 18) A \rightarrow X and Ultraviolet Systems,
M. Kimura and Y. Uchida,
Sci. Papers Inst. Phys. Chem. Res. 18, 109-18
- (32. 19) Ultraviolet Systems,
H. Kuhn,
Z. Physik 76, 782-92
- (33. 20) A \approx X System, Vibrational Analysis,
W. R. Fredrickson and C. R. Stannard,
Phys. Rev. 44, 632-7
- (33. 21) A \approx X System, Deperturbation Analysis,
V. Kondratjew and L. Polak,
Phys. Z. Sowjetunion 4, 764-86
- (37. 22) Ultraviolet Systems,
H. Yoshinaga,
Proc. Phys. -Math. Soc. Japan 19, 847-59
- (37. 23) Ultraviolet Systems,
H. Yoshinaga,
Proc. Phys. -Math. Soc. Japan 19, 1073-83

- (37. 24) C. H. D. Clark,
Trans. Faraday Soc. 33, 1398-401
- (38. 25) Fluorescence,
P. Pringsheim,
Physica, Pays-Bas 5, 489-94
- (40. 26) Theory,
G. B. B. M. Sutherland,
J. Chem. Phys. 8, 161-4
- (40. 27) Theory,
R. F. Barrow,
Trans. Faraday Soc. 36, 624-5
- (40. 28) Theory,
C. H. D. Clark,
Trans. Faraday Soc. 36, 370-6
- (41. 29) Theory,
H. M. Hulbert and J. O. Hirschfelder,
J. Chem. Phys. 9, 61-9
- (47. 30) Preliminary Note to (49.33),
R. W. B. Pearse and S. P. Sinha,
J. Phys. Soc. 160, 159
- (47. 31) Ultraviolet Systems, C \approx X System,
S. P. Sinha,
Proc. Phys. Soc. A 59, 610-21
- (49. 32) S. P. Sinha,
Indian J. Phys. 23, 229-36
- (49. 33) C \approx X System, Vibrational Analysis,
S. P. Sinha,
Proc. Phys. Soc. A 62, 124-30
- (50. 34) G. S. Chang,
Chinese J. Phys. 7, 377-82
- (60. 35) D, C - X Systems,
R. F. Barrow, N. Travis, and C. V. Wright,
Nature 187, 141-2
- (64. 36) Magnetic Moment,
R. A. Brooks, C. H. Anderson, and N. F. Ramsey,
Phys. Rev. 136, 62-8

- (65. 37) RKR Potential Curves, Dissociation Energy,
R. B. Singh and D. K. Rai,
Indian J. Pure Appl. Phys. 3, 475-8
- (66. 38) L. Szasz and G. McGinn,
"Atomic and Molecular Calculations With the Pseudopotential Method.
I. The Binding Energy and Equilibrium Internuclear Distance of the
Na₂ Molecule,"
J. Chem. Phys. 45, 2898-2912
- (68. 39) L. Szasz and G. McGinn,
"Atomic and Molecular Calculations With the Pseudopotential Method.
III. The Theory of Li₂, Na₂, K₂, LiH, NaH, and KH,"
J. Chem. Phys. 48, 2997-3008
- (69. 40) D. C. Jain and R. C. Sahni,
"Reduced Potential Energy Curves of Some Electronic States of
Alkali Molecules,"
Trans. Faraday Soc. 65, 897-903
- (69. 41) W. Demtröder, M. McClintock, and R. N. Zare,
"Spectroscopy of Na₂ Using Laser-Induced Fluorescence,"
J. Chem. Phys. 51, 5495-5508
- (69. 42) P. L. Goodfriend,
"Estimation of Spectroscopic Trends by a Perturbation Method Using
Hellmann Psuedopotentials,"
J. Molec. Spectrosc. 30, 111-5
- (69. 43) M. McClintock, W. Demtröder, and R. N. Zare,
"Level-Crossing Studies of Na₂ Using Laser-Induced Fluorescence,"
J. Chem. Phys. 51, 5509-21
- (70. 44) S. E. Johnson, K. Sakurai, and H. P. Broida,
"Fluorescence of Na₂ Induced by a Helium-Neon Laser at 632. 8 and
640. 1 nm,"
J. Chem. Phys. 52, 6441-2
- (70. 45) A. C. Roach and P. Baybutt,
"Potential Curves of Alkali Diatomic Molecules and the Origins of
Bonding Anomalies,"
Chem. Phys. Letters 7, 7-10
- (70. 46) G. Baumgartner, W. Demtröder, and M. Stock,
"Lifetime-Measurements of Alkali-Molecules Excited by Different
Laserlines,"
Z. Physik 232, 462-72

- (71. 47) K. Bergmann and W. Demtröder,
"Inelastic Collision Cross Section of Excited Molecules. I. Rotational Energy Transfer Within the B¹Π_u-State of Na₂ Induced by Collisions with He,"
Z. Physik 243, 1-13
- (71. 48) W. S. Struve, T. Kitagawa, and D. R. Herschbach,
"Chemiluminescence in Molecular Beams: Electronic Excitation in Reactions of Cl Atoms With Na₂ and K₂ Molecules,"
J. Chem. Phys. 54, 2759-61
- (71. 49) P. P. Sorokin and J. R. Lankard,
"Emission Spectra of Alkali-Metal Molecules Observed With a Heat-Pipe Discharge Tube,"
J. Chem. Phys. 55, 3810-3
- (72. 50) A. C. Roach,
"Theoretical Ground State and Excited State Potential Energy Curves for Alkali Diatomic Molecules,"
J. Molec. Spectrosc. 42, 27-37
- (72. 51) K. Bergmann and W. Demtröder,
"Inelastic Collision Cross Section of Excited Molecules. II. Asymmetries in the Cross Section for Rotational Transitions in the Na₂ (B¹Π_u) State,"
J. Phys. B 5, 1386-95
- (72. 52) K. Bergmann and W. Demtröder,
"Inelastic Cross Sections of Excited Molecules. III. Absolute Cross Sections for Rotational and Vibrational Transitions in the Na₂(B¹Π_u) State,"
J. Phys. B 5, 2098-106
- (72. 53) K. Bergmann, H. Klar, and W. Schlecht,
"Asymmetries in Collision-Induced Rotational Transitions,"
Chem. Phys. Letters 12, 522-5
- (74. 54) R. H. Callender, J. I. Gersten, R. W. Leigh, and J. L. Yang,
"Dependence of Transition Moment on Internuclear Separation in Na₂,"
Phys. Rev. Letters 32, 917-20
- (74. 55) R. W. Molof, T. M. Miller, H. L. Schwartz, B. Bederson, and J. T. Park,
"Measurements of the Average Electric Dipole Polarizabilities of the Alkali Dimers,"
J. Chem. Phys. 61, 1816-22

Na₂

- (74. 56) M. M. Hessel, E. W. Smith, and R. E. Drullinger,
"Transition Dipole Moment of Na₂ and Its Variation With Internuclear
Distance,"
Phys. Rev. Letters 33, 1251-4

Nd₂Spectroscopic Constants

Dissociation energy = 0.82 ± 0.30 eV, 19 kcal/mole, 6614 cm^{-1} (72.1).

Nd₂

BIBLIOGRAPHY

- (72. 1) A. Kant and S. Lin,
"Dissociation Energies of the Homonuclear Diatomic Molecules of
the Rare Earths,"
Monatshefte für Chemie 103, 757-63

Ne₂Methods of Production and Experimental Technique

Absorption.

Discharge.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	I	$A(\zeta_u^+) \rightarrow X^1\Sigma_g^+(0^+)$	Absorption	747-745	V			(72.5)
	II	$B(0_u^+) \rightarrow X^1\Sigma_g^+$	Absorption	737-736	V			(72.5)
	III	$C(1_u) \rightarrow X^1\Sigma_g^+$	Absorption	639-630				(72.5)
	IV	$D(0_u^+) \rightarrow X^1\Sigma_g^+$	Absorption	631-629				(72.5)
	V	$E(0_u^+) \rightarrow X^1\Sigma_g^+$	Absorption	628-626				(72.5)
	VI	$F(0_u^-)? \rightarrow X^1\Sigma_g^+$	Absorption	629-627				(72.5)
	VII	$G(0_u^+) \rightarrow X^1\Sigma_g^+$	Absorption	624-619				(72.5)
	VIII	$H(0_u^+) \rightarrow X^1\Sigma_g^+$	Absorption	624-619				(72.5)
	IX	$I(0_u^+) ? \rightarrow X^1\Sigma_g^+$	Absorption	618-615				(72.5)
	X	$J(1_u) \rightarrow X^1\Sigma_g^+$	Absorption	609-603				(72.5)
	XI	$K(0_u^+) \rightarrow X^1\Sigma_g^+$	Absorption	604-602				(72.5)

Molecule Ne₂

Ne₂

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography
	XII	$L(0_u^+, 0_u^-) -$	Absorption	601-600				(72.5)

Molecule Ne₂

I. $A(0_u^+) \leftarrow X^1\Sigma_g^+(0_g^+)$ SystemBand heads, λ (Intensity) (72.5):

(v', v'')	$(v, 0)$	$(v-1, 0)$	$(v-2, 0)$	$(v-3, 0)$
λ	745.11	745.34	745.85	746.83
(Intensity)	10	3	4	0

II. $B(0_u^+) \leftarrow X^1\Sigma_g^+$ SystemBand heads, λ (Intensity) (72.5):

(v', v'')	$(v, 0)$	$(v, 1)$	$(v-1, 0)$	$(v-1, 1)$
λ	736.18	736.25	736.49	736.57
(Intensity)	10	8	3	1

III. $C(1_u) \leftarrow X^1\Sigma_g^+$ SystemBand heads, λ (Intensity) (72.5):

(v', v'')	$(v, 0)$	$(v-1, 0)$	$(v-2, 0)$	$(v-3, 0)$	$(v-4, 0)$	$(v-5, 0)$
λ	630.98	631.49	632.05	632.71	633.45	634.26
(Intensity)	10	9	8	6	4	2

VI. $D(0_u^+) \leftarrow X^1\Sigma_g^+$ SystemBand heads, λ (Intensity) (72.5):

(v', v'')	$(v, 0)$	$(v-1, 0)$	$(v-2, 0)$
λ	629.87	630.06	630.27
(Intensity)	4	6	10

V. $E(0_u^+) \leftarrow X^1\Sigma_g^+$ SystemBand heads, λ (Intensity) (72.5):

(v', v'')	$(v, 0)$	$(v-1, 0)$	$(v-2, 0)$	$(v-3, 0)$
λ	626.92	627.03	627.23	627.46
(Intensity)	2	5	6	10

VI. F(0_u⁻) ← X¹Σ_g⁺ System

Band heads, λ (Intensity) (72.5):

(v', v'')	(v, 0)	(v-1, 0)	(v-2, 0)	(v-2, 1)	(v-3, 0)
λ	619.26	619.62	620.07	620.13	620.61
(Intensity)	10	7	6	2	5

VII. G(0_u⁺) ← X¹Σ_g⁺ System

Band heads, λ (Intensity) (72.5):

(v', v'')	(v, 0)	(v-1, 0)	(v-2, 0)	(v-3, 0)
λ	619.42	619.80	620.28	620.82
(Intensity)	10	7	4	2

VIII. H(0_u⁺) ← X¹Σ_g⁺ System

Band heads, λ (Intensity) (72.5):

(v', v'')	(v, 0)	(v-1, 0)	(v-2, 0)	(v-3, 0)
λ	619.42	619.80	620.28	620.82
(Intensity)	10	7	4	2

IX. I(0_u⁺) ← X¹Σ_g⁺ System

Band heads, λ (Intensity) (72.5):

(v', v'')	(v, 0)	(v-1, 0)	(v-2, 0)	(v-3, 0)
λ	616.30	616.53	616.81	617.06
(Intensity)	10	5	8	3

X. J(1_u) ← X¹Σ_g⁺ System

Band heads, λ (Intensity) (72.5):

(v', v'')	(v-1, 0)	(v-2, 0)	(v-3, 0)	(v-4, 0)
λ	603.57	603.85	604.28	604.74
(Intensity)	10	8	7	7

XI. K(0_u^+) - X(1_g^+) System

Band heads, λ (Intensity) (72.5):

(v' , v'')	(v , 0)	($v-1$, 0)	($v-2$, 0)	($v-3$, 0)	($v-4$, 0)
λ	602.88	602.90	602.97	603.08	603.23
(Intensity)	6	4	5	6	10

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e \omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$X^1\Sigma_g^+$	0	31.3	6.84	0.20	60		2.91		(72.5)
Dissociation energy = 3.74×10^{-3} eV, 10.6 cal/mole, 30.2 cm^{-1} (72.5).									

Perturbations and General Information

Radiative lifetimes - calculated (74.15):

$$i_u(3P_2) \rightarrow X^1\Sigma_g^+ \quad \tau = 11.9 \mu\text{sec}$$

$$0_u^+(3P_1) \rightarrow X^1\Sigma_g^+ \quad \tau = 2.8 \text{ nsec}$$

$$0_u^+(1P_1) \rightarrow X^1\Sigma_g^+ \quad \tau = 1.2 \text{ nsec}$$

BIBLIOGRAPHY

- (58. 1) Observation of Ultraviolet Continuum,
Y. Tanaka, A. S. Jursa, and F. J. LeBlanc,
J. Opt. Soc. Am. 48, 304-8
- (67. 2) J. F. Prince and W. W. Robertson,
"Visible Continua in Xenon, Krypton, and Neon,"
J. Chem. Phys. 46, 3309-13
- (67. 3) Theory,
T. L. Gilbert and A. C. Wahl,
J. Chem. Phys. 47, 3425-38
- (67. 4) P. G. Wilkinson,
The Mechanism of the Argon Emission Continuum in the Vacuum
Ultraviolet,"
Can. J. Phys. 45, 1715-27
- (72. 5) Y. Tanaka and K. Yoshino,
"Absorption Spectra of Ne₂ and HeNe Molecules in the Vacuum-uv
Region,"
J. Chem. Phys. 57, 2964-76
- (72. 6) D. D. Konowalow, P. Weinberger, J. L. Calais, and J. W. D. Connolly,
"Self-Consistent-Field $\times \alpha$ Cluster Calculations for the Ground State
Ne₂ Molecule,"
Chem. Phys. Letters 16, 81-5
- (73. 7) G. C. Maitland,
"The Determination of the Intermolecular Potential Energy Function
of Neon From Spectroscopic, Equilibrium and Transport Data,"
Molec. Phys. 26, 513-28
- (73. 8) J. M. Farrar, Y. T. Lee, V. V. Goldman, and M. L. Klein,
"Neon Interatomic Potentials From Scattering Data and Crystalline
Properties,"
Chem. Phys. Letters 19, 359-62
- (73. 9) M. L. Klein,
"Comments on the Interatomic Potential of Ne₂,"
Chem. Phys. Letters 18, 203-4
- (73. 10) Y. Tanaka, K. Yoshino, and D. E. Freeman,
"On the Determination of the Ground State Potential Energy of Ne₂
From its Vacuum Ultraviolet Spectrum,"
J. Chem. Phys. 59, 564-5

- (74. 11) W. J. Stevens, A. C. Wahl, M. A. Gardner, and A. M. Karo,
"Ab Initio Calculation of the Neon-Neon $1\Sigma_g^+$ Potential at Intermediate
Separations,"
J. Chem. Phys. 60, 2195-7
- (74. 12) R. J. LeRoy, M. L. Klein, and I. J. McGee,
"On the Dissociation Energy and Interaction Potential of Ground-
State Ne₂,"
Molec. Phys. 28, 587-91
- (74. 13) A. Conway and J. N. Murrell,
"The Exchange Energy Between Neon Atoms,"
Molec. Phys. 27, 873-8
- (74. 14) J. S. Cohen and B. Schneider,
"Ground and Excited States of Ne₂ and Ne₂⁺. I. Potential Curves
With and Without Spin-Orbit Coupling,"
J. Chem. Phys. 61, 3230-9
- (74. 15) B. Schneider and J. S. Cohen,
"Ground and Excited States of Ne₂ and Ne₂⁺. II. Spectroscopic
Properties and Radiative Lifetimes,"
J. Chem. Phys. 61, 3240-3

Ni₂

Ni₂

Spectroscopic Constants

Dissociation energy = 2.37 ± 0.22 eV, 54.5 kcal/mole, 19100 cm^{-1} (64.1).

BIBLIOGRAPHY

- (64. 1) Dissociation Energy,
A. Kant,
J. Chem. Phys. 41, 1872-6

Methods of Production and Experimental Technique

Absorption: in high frequency discharges, pulsed discharges, ac discharges, flash photolysis.

Emission: all types of discharges, flames, explosions, luminescence.

In astrophysics.

Ground state studied by microwave spectroscopy.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, 0, 0	Remarks	Bibliography
Infrared atmospheric Atmospheric Noxon II Herzberg II Herzberg III, High pressure	I	$a^1\Delta_g \rightarrow X^3\Sigma_g^-$	Absorption, emission	15800-9240	R	7882.39		(72.73, 62.39, 59.32, 58.29, 47.14, 33.6)
	II	$b^1\Sigma_g^+ \rightarrow X^3\Sigma_g^-$	Absorption, emission	9970-5380	R	13120.9085		(72.73, 69.57, 64.41, 61.36, 50.18, 49.17)
	III	$b^1\Sigma_g^+ \rightarrow a^1\Delta_g$	Discharge	19080		5240 (head)	Only a single band	(69.57)
	IV	$c^1\Sigma_u^- \rightarrow X^3\Sigma_g^-$	Absorption, lumines- cence	4790-4490 2715-2540	R	32664.1 (calculated)		(68.49, 53.22)
	V	$C^3\Delta_u \rightarrow X^3\Sigma_g^-$	Absorption at high pressure	2630-2570 2924-2440	R	34319 (head)		(53.22, 39.11, 34.8, 32.5, 28.1)

Molecule O₂

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
Chamberlain Herzberg I Schumann- Runge	VI	$C^3\Delta_u \rightarrow a^1\Delta_g$	Lumines- cence	4380-3700	R			(58.27)
	VII	$A^3\Sigma_u^+ \rightarrow X^3\Sigma_g^-$	Absorption, lumines- cence	4880-2430	R	35007.15 (calculated)		(60.33, 59.31, 57.26, 55.25)
	VIII	$B^3\Sigma_u^- \rightarrow X^3\Sigma_g^-$	All sources	5350-1750 1750-1300	R Continuum	49358.15		(72.73, 68.54, 68.52, 66.45, 64.43, 64.42, 61.35, 59.30, 54.24, 54.23, 50.19)
	IX	$\alpha^1\Sigma_u^+ \rightarrow b^1\Sigma_g^+$		1585-1538	V	63141.5		(68.48)
		$\alpha^1\Sigma_u^+ \rightarrow X^3\Sigma_g^-$		1280-1196	V			(69.58, 68.48)
		$\beta^3\Sigma_u^+ \rightarrow X^3\Sigma_g^-$	Absorption	1294-1181	V			(69.58, 68.48, 52.21)
		$1\Delta_u \rightarrow a^1\Delta_g$		1243.8 (only a single band)		80396.0		(68.48)

Molecule
O₂

Molecule O₂

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
Rydberg Series	IX (cont)	$1\Pi_u \rightarrow a^1\Delta_g$		1229.0 (only a single band)		81362.5		(68.48)
		$3\Sigma_u^+ \rightarrow X^3\Sigma_g^-$		1144.6 (only a single band)	V	87369.1		(69.58)
	X	$X^2\Pi_g(0_2^+) \rightarrow X^3\Sigma_g^-$		1290-1180	V			(61.38, 52.21)
		$b^4\Sigma_g^-(0_2^+) \rightarrow X^3\Sigma_g^-$	Absorption	730-660	R			(68.51, 33.9)
		$B^2\Sigma_g^-(0_2^+) \rightarrow X^3\Sigma_g^-$		650-600	R			(68.51, 68.50, 42.12)
		$c^4\Sigma_u^-(0_2^+) \rightarrow X^3\Sigma_g^-$		595-510				(69.61)
	XI	Many bands that are unclassified or whose identification is doubtful						(68.51, 68.48, 67.47, 61.37, 54.24, 52.21, 48.16, 43.13)

Molecule O₂

I. $a^1\Delta_g \rightleftharpoons X^3\Sigma_g^-$ System (Infrared Atmospheric)

Band origins, λ (58.29, 47.14, 33.6):

(v', v'')	(0, 1)	(0, 0)	(1, 0)	(2, 0)
λ	(15800)	1263.0	10674.1	(9240)

II. $b^1\Sigma_g^+ \rightleftharpoons X^3\Sigma_g^-$ System (Atmospheric)

Band heads in emission, λ (69.57, 64.41, 61.36, 50.18, 49.17):

v', v''	0	1	2	3	4
0	7593.73	(8623)	(9970)		
1	6867.2	7683.85	8697.8		
2	6276.6	6953	7779.03		
3			7043	7879.17	
4				7141	7987

III. $b^1\Sigma_g^+ \rightarrow a^1\Delta_g$ System (Noxon)

Only a single band, Q branch (69.57):

$\lambda(0, 0) | 19080$

IV. $c^1\Sigma_u^- \rightleftharpoons X^3\Sigma_g^-$ System (Herzberg II)

Band origins (calculated), λ (68.49):

v', v''	0	1	2	3	4	5	6	7	8
0	3060.6	3213.7	3380.3	3562.0	3761.2	3980.3	4222.4	4491.2 ^(a)	4791.5 ^(a)
1	2990.3	3136.3	3294.7	3467.2	3655.6	3862.2	4089.7	4341.5	4621.4
2	2925.5	3065.1	3216.2	3380.4	3559.2	3754.8	3969.5	4206.2	4468.5
3	2865.8	2999.7	3144.3	3301.0	3471.3	3657.1	3860.5	4084.0	4330.8
4	2811.0	2939.6	3078.4	3228.4	3391.1	3568.2	3761.6	3973.5	4206.7
5	2760.6	2884.6	3018.1	3162.1	3318.1	3487.5	3671.9	3873.6	4094.9
6	2714.5 ^(b)	2834.2	2963.0	3101.8	3251.7	3414.2	3590.8	3783.4	3994.2
7	2672.3 ^(b)	2788.3	2912.9	3046.9	3191.4	3347.8	3517.4	3702.0	3903.6
8	2634.0 ^(b)	2746.6	2867.4	2997.1	3136.9	3287.8	3451.3	3628.8	3822.4
9	2599.2 ^(b)	2708.9	2826.2	2952.2	3087.7	3233.9	3391.9	3563.2	3749.6
10	2568.0 ^(b)	2674.9	2789.3	2911.9	3043.7	3185.6	3338.8	3504.7	3684.9

(a) Observed in luminescence, (b) observed in absorption (53.22)

V. $C^3\Delta_u \leftarrow X^3\Sigma_g^-$ System (Herzberg III, High Pressure Bands)

Herzberg III

Two fragments with three heads have been observed (53.24).
Vibrational numbering is uncertain.

(v', v'')	$F_2(6, 0)$	$F_3(6, 0)$	$(5, 0)$
λ	2589.14	2579.39	2620.71

High Pressure Bands (diffuse)

Maxima in absorption (no heads), λ (39.11).
Vibrational numbering is uncertain.

(v', v'')	(0,0)	(1,0)	(2,0)	(3,0)	(4,0)	(5,0)	(6,0)	(7,0)	(8,0)	(9,0)
λ	2924	2855	2795	2739.8	2689.8	2642.7	2598.8	2555.9	2525.4	2497.4
	2913	2842	2783.9	2729.9	2679.3	2632.7	2590.3	2553.5	2517	2488.7
	2904	2832	2769.1	2720.7	2671.6	2626	2582.4	2537	2510	2482

VI. $C^3\Delta_u \rightarrow a^1\Delta_g$ System (Chamberlain)

27 weak bands have been observed, but the identification is uncertain.
Vibrational numbering of the lower state is uncertain.

Possible band heads, λ (53.24):

			$^3\Delta_1$			
v', v''	0	1	2	3	4	5
0						
1			4135			
2						
3			3887	4114		
4					4244	
5			3698		4127	4378
6				3813	4031	

v', v''	0	1	$\frac{3}{2}\Delta_2$	3	4	5
			2			
0						
1			4107			
2						
3			3866	4090		
4					4221	
5					4107	
6				3792	4009	4240

v', v''	0	1	$\frac{3}{2}\Delta_3$	3	4	5
			2			
0						
1			4086			
2						
3			3844	4071	4317	
4						
5				3861	4086	4326
6				3771	3985	4215

VII. $A^3\Sigma_u^+ \rightleftharpoons X^3\Sigma_g^-$ System (Herzberg I)

Band heads in emission, λ (Intensity) (59.21):

v', v''	0	1	2	3	4	5	6	7	8
0							3840 (5)	4064 (5)	4309 (7)
1					(3366.5) (2)	3542 (8)	3734 (8)	3938 (7)	4170 (6)
2					3285 (7)	3453 (8)	3633 (8)	3829 (8)	4044 (2)
3			2931 (1)	3066 (5)	3211 (10)	3370 (10)	3542 (8)	(3726.1) (2)	(3842.2) (2)
4			2873 (2)	3002 (5)	3142 (7)	3292 (4)	3459 (2)	(3634.6) (2)	
5			2820 (3)	2945 (5)	3080	(3225.0) (2)		(3552.5) (4)	(3737.7) (4)
6			2775 (3)	2895 (6)	3026 (2)		(3315.7) (2)	(3479.3) (4)	3657 (2)
7		2622 (3)	2734 (5)	2850 (5)			(3257.1) (4)	(3414.7) (4)	
8		2588 (2)	2696 (4)						

VIII. $B^3\Sigma_u^- \rightleftharpoons X^3\Sigma_g^-$ System (Schumann-Runge)

Band origins in absorption, λ (68.54, 66.45, 64.43, 64.42, 59.30, 54.23, 50.19):

v', v''	0	1	2	3	4	5	6	7	8
0	2026.01								
1	1998.17							2522.67	2614.67
2	1971.97	2034.29				2316.82	2396.80	2481.02	2569.95
3	1947.33	2008.11				2282.89	2360.52	2442.25	
4	1924.19	1983.60		2110.91	2179.36	2251.21	2326.53		
5	1902.23	1960.58	2021.28	2084.93	2151.61	2221.53	2295.03		
6	1882.43	1939.25	1998.63	2060.84	2125.94	2194.20			
7	1863.72	1919.37	1977.57	2038.35	2102.05	2168.78			
8	1846.51	1901.14	1958.21	2017.84	2080.22	2145.54			
9	1830.76	1884.47	1940.47	1999.05	2060.27	2124.31			
10	1816.50	1869.37	1924.48	1982.02	2042.23	2105.05			

IX. Partial Systems $\alpha^1\Sigma_u^+ \leftarrow b^1\Sigma_g^+$ SystemBand heads, λ (68.48):

(v', v'')	(0, 0)	(1, 1)	(1, 0)
λ	1583.9	1571.9	1537.9

 $\alpha^1\Sigma_u^+ \leftarrow X^3\Sigma_g^-$ SystemBand heads, λ (69.58, 68.48):

(v', v'')	(1, 0)	(2, 0)	(3, 0)	(4, 0)
λ	1279.5	1250.0	1222.1	1196.4

 $\beta^3\Sigma_u^+ \leftarrow X^3\Sigma_g^-$ SystemBand origins, λ (69.58, 68.48):

(v', v'')	(2, 0)	(3, 0)
λ	1262.18	1233.47

 $^1\Delta_u \leftarrow a^1\Delta_g$ SystemBand head, λ (68.48):

(v', v'')	(0, 0)
λ	1243.8

 $^1\Pi_u \leftarrow a^1\Delta_g$ SystemBand head, λ (68.48):

(v', v'')	(0, 0)
λ	1229.0

${}^3\Sigma_u^+ \leftarrow X{}^3\Sigma_g^-$ System

Double headed bands with 3 branches. Band head, λ (69.58):

$$\begin{array}{cc} (v', v'') & (0, 0) \\ \lambda & 1144.6 \end{array}$$

X. Rydberg Series

$X{}^2\Pi_g(0_2^+) \leftarrow X{}^3\Sigma_g^-$ System

Single progression of doublets. Classification is doubtful (61.38, 52.21).

$b{}^4\Sigma_g^-(0_g^+) \leftarrow X{}^3\Sigma_g^-$ System

Many progressions with the proposed configuration $\dots np \sigma_u {}^3\Sigma_u$ have been observed (68.38, 62.40, 35.9).

Band head formula: $\nu = 146568 - \frac{R}{(n-1.679)^2} \quad (n = 5 \dots \infty)$

Another weak, diffuse series has been observed with a proposed configuration of $np \pi_u {}^3\Pi_u$ (68.38).

$B{}^2\Sigma_g^-(0_2^+) \leftarrow X{}^3\Sigma_g^-$ System

Bands with simple heads (68.51, 68.50, 42.12).

Band head formula: $\nu = 163602 - \frac{R}{(n-0.658)^2} \quad (n = 4 \dots \infty)$

c⁴Σ_u⁻(0₂⁺) ← X³Σ_g⁻ System

Several series have been observed (69.61).

Π Series - probably excited to the nd π_g ³Π_u Rydberg state.

$$\text{Band head formula: } \nu = 198125 - \frac{R}{(n-1.559)^2} \quad (n=4 \cdots \infty)$$

Σ Series - probably excited to the ns σ_g ³Σ_u⁻ Rydberg state.

$$\text{Band head formula: } \nu = 198125 - \frac{R}{(n-0.955)^2} \quad (n=4 \cdots \infty)$$

SPECTROSCOPIC CONSTANTS

Molecule O₂

State	T _e	ω _e	x _e ω _e	B _e	α _e × 10 ²	D _e × 10 ⁶	r _e	Remarks	Bibliography
¹ Π _u	89244.9(a)			(1.451)					(68.48)
¹ Δ _u	88278.4(a)			(1.446)					(68.48)
³ Σ _u ⁺	87369.1(a)			(1.706)	(2800)				(69.58)
^α ¹ Σ _u ⁺	76089	(1927)	(19)	1.599	1.6				(69.58, 68.48)
^β ³ Σ _u ⁺	75263	(1957)	(19.7)	(1.7)	(2)				(69.58, 68.48, 52.21)
^B ³ Σ _u ⁻	49794.33	709.058	10.6141	0.818975	1.19225		1.60428	(b, g)	(70.63, 66.45, 54.23, 34.7)
^A ² Σ _u ⁺	35398.70	799.08	12.16	0.91053	1.416	4.79	1.52153	(c, h)	(54.24, 52.20)
^C ³ Δ _{u,i}	34735	(750)	(14)				(1.5)		(53.22, 39.11, 32.5)
^c ¹ Σ _u ⁻	33058.4	794.29	12.736	0.9155	1.391	(10.5)	1.5174	(d, i)	(68.49, 53.22)
^b ¹ Σ _g ⁺	13195.314	1432.66	13.9336	1.4004796	1.8169303	5.356	1.22684	(e, j)	(n.p. 175, 48.15)
^a ¹ Δ _g	7918.11	(1509.3)	(12.9)	1.4263	1.71	(4.97)	1.21567		(47.14)

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e \omega_e$	B_e	$\alpha_e \times 10^2$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$X^3\Sigma_g^-$	0	1580.19	11.981	1.445622	1.593268		1.20754	(f, k)	(n.p. 125, 66.45, 54.23, 34.7)
<p>(a) T_o; (b) $y_{ew} = -0.059212435$, $z_{ew} = -0.023974994$; (c) $y_{ew} = -0.550$; (d) $y_{ew} = -0.2444$, $z_{ew} = 0.00055$;</p> <p>(e) $y_{ew} = -0.0143$; (f) $y_{ew} = 0.047474736$, $z_{ew} = -0.00012727481$; (g) $y_e = -6.30472 \times 10^{-4}$;</p> <p>(h) $y_e = -9.7 \times 10^{-4}$, $\beta_e = 3.0 \times 10^{-7}$; (i) $y_e = -7.40 \times 10^{-4}$; (j) $y_e = -4.2941920 \times 10^{-5}$, $\beta_e = 0.077$;</p> <p>(k) $y_e = 6.406456 \times 10^{-5}$</p> <p>Dissociation energy = 5.12 ± 0.0019 eV, 117.97 kcal/mole, 41260 cm^{-1} (54.23).</p>									

Perturbations and General Information

Ionization potential (I_p) to $X^2\Pi_{g,i}(0_2^+)$ = 12.059 ± 0.001 eV (68.53, 66.44).

$A^3\Sigma_u^+ - X^3\Sigma_g^-$ has a strong perturbation in the (11,0) band for $N > 11$ (52.20).

$B^3\Sigma_u^-$ state is perturbed at $v = 16$, $J = 8$ and $v = 19$, $J = 8$ (54.23).

$B^3\Sigma_u^-$ state is predissociated, probably by a repulsive $^3\Pi_u$ state. The predissociation is characterized by an onset at $v = 2$ and broadening at $v = 4, 8$, and 11 , with a minimum at $v = 9$. The interpretation of the predissociation is in question (72.73, 70.62, 69.60, 69.59, 61.36, 59.30, 58.28, 36.10).

Vibrational Raman effect has been observed (60.33, 30.3, 29.2).

Rotational Raman effect has been observed (74.114, 60.33, 30.3).

Potential energy curves - RKR potentials (72.73 and references cited therein):

State	v	$V(\text{cm}^{-1})$	$r_{\min}(\text{\AA})$	$r_{\max}(\text{\AA})$
$X^3\Sigma_g^-$ $T_e = 0 \text{ cm}^{-1}$	0	787.3818	1.1590417	1.2626908
	1	2343.7613	1.1272513	1.3078976
	2	3876.57	1.10700	1.34170
	3	5386.03	1.09146	1.37093
	4	6872.34	1.07864	1.39759
	5	8335.65	1.06767	1.42257
	6	9776.11	1.0580	1.4464
	7	11193.80	1.0494	1.4693
	8	12588.82	1.0417	1.4917
	9	13961.18	1.0346	1.5136
	10	15310.91	1.0280	1.5351
$a^1\Delta_g$ $T_e = 7918.11 \text{ cm}^{-1}$	0	751.658	1.16619	1.27228
	1	2235.158	1.13396	1.31904
	2	3692.86	1.11353	1.35422
	3	5124.76	1.0979	1.3848
$b^1\Sigma_g^+$ $T_e = 13195.314 \text{ cm}^{-1}$	0	712.9766	1.176241	1.285186
	1	2117.7290	1.143442	1.333696
	2	3494.4855	1.122734	1.370428
	3	4843.1603	1.106952	1.402561

State	v	V(cm ⁻¹)	r _{min} (Å)	r _{max} (Å)
A ³ Σ _u ⁺ T _e = 35398.70 cm ⁻¹	0	395.8	1.454	1.600
	1	1168.7	1.411	1.668
	2	1912.5	1.385	1.722
	3	2623.5	1.366	1.772
	4	3298.9	1.350	1.822
	5	3934.9	1.337	1.872
	6	4527.2	1.326	1.925
	7	5070.0	1.317	1.982
	8	5555.6	1.310	2.050
	9	5973.4	1.304	2.131
	10	6309.1	1.298	2.245
B ³ Σ _u ⁻ T _e = 49794.33 cm ⁻¹	0	351.204	1.53266	1.68771
	1	1038.736	1.48649	1.75876
	2	1703.961	1.45776	1.81426
	3	2345.774	1.43623	1.86450
	4	2962.845	1.41889	1.91257
	5	3553.643	1.40434	1.96005
	6	4118.425	1.39181	2.00806
	7	4649.207	1.38084	2.05761
	8	5149.746	1.37117	2.10976
	9	5615.548	1.36264	2.16578
	10	6043.932	1.35518	2.22722
	11	6432.167	1.34876	2.29602

Radiative lifetimes, Einstein coefficients and oscillator strengths:

Transition	Band	$\tau(\text{sec})$	$A_{v'}$ (sec^{-1})	$A_{v'v''}$ (sec^{-1})	Absorption f -Value	Reference
$a^1\Delta_g - X^3\Sigma_g^-$	0-0	$3.88(10^3)$		$2.58(10^{-4})$	$4.15(10^{-12})$	(68.55)
$b^1\Sigma_g^+ - X^3\Sigma_g^-$	0-0			0.085	$2.47(10^{-10})$	(67.46)
	1-0			(0.0069)		(32.4)
	2-0			$(0.1636) 10^{-3}$		(68.56)
	1-1			0.0704		(68.56)
$b^1\Sigma_g^+ - a^1\Delta_g$	0-0			$1.5(10^{-3})$		(61.34)
$A^3\Sigma_u^+ - X^3\Sigma_g^-$		$(1 - 10^3)$				(67.46, 64.41, 62.40)
	7-0				$1.24(10^{-10})$	(70.64)
$c^1\Sigma_u^- - X^3\Sigma_g^-$			$\sim 10^{-4}$			(62.40)
		$> 10^{-3}$				(64.41)
$C^3\Delta_u - X^3\Sigma_g^-$			$\leq 10^{-5}$			(62.40)
		$> 10^{-3}$				(64.41)

Absolute f -values for the $B^3\Sigma_u^- - X^3\Sigma_g^-$ bands (72.73 and references cited therein):

v', v''	0	1	2
0	3.45-10		
1	3.90-9		
2	2.38-8	5.35-7	
3	9.90-8	2.08-6	
4	3.21-7	6.15-6	
5	8.52-7	1.53-5	
6	1.91-6	3.15-5	2.13-4
7	3.81-6	5.78-5	3.39-4
8	6.68-6	9.40-5	5.46-4
9	1.06-5	1.38-4	9.87-4
10	1.57-5	1.91-4	1.03-3
11	2.09-5	2.38-4	1.04-3
12	2.53-5	2.73-4	1.22-3
13	2.88-5	2.93-4	1.04-3
14	3.03-5	2.95-4	
15	2.92-5	2.77-4	
16	2.59-5	2.42-4	
17	2.23-5	2.01-4	
18	1.83-5		
19	1.44-5		

f -value followed by a factor of ten

Franck-Condon factors - RKR potentials (n.p. 125, 72.73):

$a^1\Delta_g - X^3\Sigma_g^-$

v', v''	0	1	2	3	4
0	9.869-1	1.297-2	1.260-4		
1	1.303-2	9.586-1	2.791-2	4.296-4	1.735-6
2	6.795-5	2.814-2	9.258-1	4.497-2	9.802-4
3	2.591-4	4.548-2	8.881-1	6.423-2	1.867-3

Franck-Condon factors followed by a factor of ten

$$\underline{b^1\Sigma_g^+ - X^3\Sigma_g^-}$$

v', v''	0	1	2	3	4	5	6
0	9.308-1	6.660-2	2.523-3	5.648-5			
1	6.647-2	7.928-1	1.322-1	8.284-3	2.736-4	6.417-6	
2	2.639-3	1.315-1	6.527-1	1.943-1	1.802-2	8.232-4	2.512-5
3	6.911-5	8.753-3	1.924-1	5.144-1	2.499-1	3.240-2	1.968-3

Franck-Condon factors followed by a factor of ten

$$\underline{A^3\Sigma_u^+ - X^3\Sigma_g^-}$$

v', v''	6	7	8	9	10	11	12
0	4.260-2	7.935-2	1.214-1	1.546-1	1.654-1	1.495-1	1.140-1
1	8.985-2	1.052-1	8.298-2	3.500-2	1.510-3	1.512-2	6.765-2
2	8.158-2	4.457-2	4.492-3	1.049-2	5.486-2	7.589-2	4.343-2
3	3.593-2	1.434-3	1.700-2	5.478-2	4.681-2	6.822-3	9.761-3
4	3.900-3	1.162-2	4.595-2	3.559-2	1.700-3	1.847-2	5.157-2

Franck-Condon factors followed by a factor of ten

$$\underline{B^3\Sigma_u^- - X^3\Sigma_g^-}$$

v', v''	12	13	14	15	16	17
0	1.192-1	1.443-1	1.514-1	1.378-1	1.087-1	7.417-2
1	6.350-2	2.328-2	3.441-4	1.553-2	6.165-2	1.087-1
2	5.507-5	1.853-2	5.696-2	6.930-2	3.928-2	3.934-3
3	3.150-2	5.446-2	3.492-2	2.823-3	1.221-2	5.283-2
4	4.503-2	1.900-2	1.904-4	2.620-2	4.910-2	2.392-2
5	1.579-2	6.553-4	2.667-2	3.844-2	9.388-3	5.262-3

Franck-Condon factors followed by a factor of ten

$$\underline{b^1\Sigma_g^+ - a^1\Delta_g}$$

v', v''	0	1	2	3
0	9.770-1	2.283-2	2.136-4	
1	2.267-2	9.290-1	4.760-2	7.217-4
2	3.628-4	4.694-2	8.768-1	7.430-2
3	4.426-6	1.213-3	7.266-2	8.202-1

Franck-Condon factors followed by a factor of ten

BIBLIOGRAPHY

References for this molecule are only those from which spectroscopic information has been taken directly and those papers published after 1970. The reason for excluding the publications from before 1971 is the reference (72.73) in our Bibliography. This publication provides a Bibliography through the beginning of 1971, as well as an excellent critical review of the O₂ molecule.

- (28. 1) Triplet Systems at High Pressure,
D. S. Villars,
Proc. Nat. Acad. Sci. 14, 508-11
- (29. 2) Vibration-Rotation Raman Effect,
F. Rasetti,
Phys. Rev. 34, 367-71
- (30. 3) Vibration-Rotation and Rotation, Raman Effect,
F. Rasetti,
Z. Physik 61, 598-601
- (32. 4) A - X System,
G. Herzberg,
Naturwissenschaften 20, 577
- (32. 5) C - X System, 2300-2900Å Bands,
W. Finkelburg and W. Steiner,
Z. Physik 79, 69-88
- (33. 6) a - X System,
J. W. Ellis and H. O. Kneser,
Z. Physik 86, 583-91
- (34. 7) B - X System, a - X System Rotational Constant,
J. Curry and G. Herzberg,
Ann. Phys. 19, 800-18
- (34. 8) Triplet System,
W. Finkelburg,
Z. Physik 90, 1-10
- (35. 9) b - X Rydberg Series and Unclassified Rydberg Series,
W. C. Price and G. Collins,
Phys. Rev. 48, 714-9

- (36. 10) Predissociation,
P. J. Flory,
J. Chem. Phys. 4, 23-7
- (39. 11) C, A - X Systems,
L. Herman,
Ann. Phys. 11, 548-611
- (42. 12) b, B - X Rydberg Series, Vibrational Structure,
Y. Tanaka and T. Takamine,
Sci. Papers Inst. Phys. Chem. Res. 39, 437-46
- (43. 13) Unclassified Rydberg Series,
N. L. Singh and L. Lal,
Sci. and Culture 9, 89
- (47. 14) a - X System, Spectroscopic Constants,
L. Herzberg and G. Herzberg,
Astrophys. J. 105, 353-9
- (48. 15) b - X System, Spectroscopic Constants of X State,
H. D. Babcock and L. Herzberg,
Astrophys. J. 108, 167-90
- (48. 16) B - X System,
L. Lal,
Nature 161, 477-8
- (49. 17) b - X System,
R. C. Herman, H. S. Hopfield, G. A. Hornbeck, and S. Silverman,
J. Chem. Phys. 17, 220-1
- (50. 18) b - X System,
A. B. Meinel,
Astrophys. J. 112, 464-8
- (50. 19) B - X System at High Temperature,
A. Herczog and K. Wieland,
Helv. Phys. Acta 23, 432-6
- (52. 20) A - X System, Spectroscopic Constants,
G. Herzberg,
Can. J. Phys. 30, 185-210
- (52. 21) α , β - X Rydberg Systems,
Y. Tanaka,
J. Chem. Phys. 20, 1728-33

- (53.22) c, C - X Systems, C - a System,
G. Herzberg,
Can. J. Phys. 31, 657-69
- (54.23) B - X System, a - X System, Spectroscopic Constants,
P. Brix and G. Herzberg,
Can. J. Phys. 32, 110-35
- (54.24) A, c - X System,
H. P. Broida and A. G. Gaydon,
Proc. Roy. Soc. A 222, 181-95
- (55.25) A - X System,
J. W. Chamberlain,
Astrophys. J. 121, 277-86
- (57.26) A - X System,
C. A. Barth and J. Kaplan,
J. Chem. Phys. 26, 506-10
- (58.27) C → a System, Spectroscopic Constants,
J. W. Chamberlain,
Astrophys. J. 128, 713-7
- (58.28) New B - X System Bands in the Ultraviolet, Predissociation,
D. Rakotoarijimy, S. Weniger, and H. Grenat,
C. R. Acad. Sci. 246, 2883-6
- (53.29) a - X System,
A. V. Jones and A. W. Harrison,
J. Atm. Terrestr. Phys. 13, 45-60
- (59.30) B - X System, Predissociation,
P. K. Carroll,
Astrophys. J. 129, 794-800
- (59.31) A - X System,
C. A. Barth and J. Kaplan,
J. Molec. Spectrosc. 3, 583-7
- (59.32) Infrared Systems,
J. Connes and H. P. Gush,
J. Phys. Radium 20, 915-7
- (60.33) Raman Spectrum,
A. Weber and E. A. MacGinnis,
J. Molec. Spectrosc. 4, 195-200

- (61. 34) b - a System, Spectroscopic Constants,
J. F. Noxon,
Can. J. Phys. 39, 1110-9
- (61. 35) B - X System,
G. R. Broert and R. W. Nicholls,
J. Atm. Terrestr. Phys. 21, 21
- (61. 36) b, B - X Systems, Predissociation,
L. Herman, R. Herman, and D. Rakotoarijimy,
J. Phys. Radium 22, 1-8
- (61. 37) Unclassified Rydberg Series,
J. Byrne,
Proc. Phys. Soc. 78, 1074-5
- (61. 38) Rydberg Series,
W. R. Jarman,
Yerkes Obs., Univ. Chicago, Sci. Report No. 35
- (62. 39) b - X System, Spectroscopic Constants,
A. Landau, E. J. Allin, and H. L. Welsh,
Spectrochim. Acta 18, 1-19
- (62. 40) 3000-12400Å Atlas,
V. I. Krossovsky, N. N. Shefov, and V. I. Yaim,
Planet. Space Sci. 9, 883-915
- (64. 41) b - X System,
J. A. Curcio, L. F. Drummeter, and G. L. Knestrick,
Appl. Opt. 3, 1401-9
- (64. 42) B - X System,
A. M. Bass and D. Garvin,
J. Chem. Phys. 40, 1772-3
- (64. 43) B - X System,
R. V. Fitzsimmons and E. J. Blair,
J. Chem. Phys. 40, 451-8
- (60. 44) Ionization Potential,
J. A. R. Samson and R. B. Cairns,
J. Opt. Soc. Am. 56, 769-75
- (66. 45) a, B - X Systems,
M. Ogawa,
Science Light 15, 97-114

- (67. 46) Line Shapes,
D. E. Burch and D. A. Gryvnak,
Appl. Opt. 8, 1493-9
- (67. 47) 830-900Å Bands,
R. E. Huffman, J. C. Larrabee, and Y. Tanaka,
J. Chem. Phys. 46, 2213-33
- (68. 48) α -b, α -X, B-X, $^1\Delta_u$ -a $^1\Delta_g$, $^1\Pi_u$ -a $^1\Delta_g$ Systems and X-X Rydberg System,
F. Alberti, R. A. Ashby, and A. E. Douglas,
Can. J. Phys. 46, 337-42
- (68. 49) c-X System,
R. K. Dhumwad and N. A. Narasimham,
Can. J. Phys. 46, 1254-5
- (68. 50) B-X Rydberg System,
M. Ogawa,
Can. J. Phys. 46, 312-3
- (68. 51) b, B-X Rydberg Systems, Unclassified Bands < 600Å, Ionization Potential,
K. Yoshino and Y. Tanaka,
J. Chem. Phys. 48, 4859-67
- (68. 52) B-X System Between 300 to 900°K,
R. D. Hudson and V. L. Carter,
J. Opt. Soc. Am. 58, 1621-9
- (68. 53) Ionization Potential,
G. L. Bhale and P. R. Rao,
Proc. Indian Acad. Sci. A 67, 350-7
- (68. 54) B-X System,
M. Ogawa and H. C. Chang,
Science Light 17, 45-56
- (68. 55) Radiative Lifetime a $^1\Delta_g$,
R. M. Badger, A. D. Wright, and R. F. Whitlock,
J. Chem. Phys. 43, 3341-63
- (68. 56) Radiative Lifetime b $^1\Sigma_g^+$,
G. F. Sitnik and A. I. Khlystov,
Izv. Atmos. Ocean. Phys. 4, 1120-2

- (69. 57) b - X System,
G. Herzberg, A. Lagerqvist, and B. J. MacKenzie,
Can. J. Phys. 47, 1889-97
- (69. 58) α , β , $^3\Sigma_u^+$ - X Systems, X - X Rydberg System, Spectroscopic
Constants,
M. Ogawa and K. R. Yamawaki,
Can. J. Phys. 47, 1805-11
- (69. 59) Predissociation,
I. Riess and Y. Ben-Aryeh,
J. Quant. Spectrosc. Radiative Trans. 9, 1463-8
- (69. 60) B - X System, Predissociation,
J. N. Murrell and J. M. Taylor,
Molec. Phys. 16, 609-21
- (69. 61) C - X Rydberg Series,
J. Hoefft, F. J. Lovas, E. Tiemann, and T. Törring,
Z. Naturforsch. A 24, 1843-4
- (70. 62) Potential Curves, Predissociation,
D. V. K. Rao and P. T. Rao,
J. Phys. B 3, 430-7
- (70. 63) B - X System,
M. Ackerman and F. Biaume,
J. Molec. Spectrosc. 35, 73-82
- (70. 64) A - X System,
V. Hasson, R. W. Nicholls, and V. Degen,
J. Phys. B 3, 1192-4
- (71. 65) T. A. Miller,
"Rotational Moment, Rotational g Factor, Electronic Orbital g
Factor, and Anisotropy of the Magnetic Susceptibility of $^1\Delta$ O₂,"
J. Chem. Phys. 54, 330-7
- (71. 66) N. Jonathan, A. Morris, K. J. Ross, and D. J. Smith,
"High Resolution Vacuum Ultraviolet Photoelectron Spectra of
Transient Species: O₂($^1\Delta_g$) and Previously Unobserved States
of O₂,"
J. Chem. Phys. 54, 4954-5
- (71. 67) F. D. Findlay and D. R. Snelling,
"Collisional Deactivation of O₂($^1\Delta_g$),"
J. Chem. Phys. 55, 545-51

- (71. 68) K. H. Becker, W. Grath, and U. Schurath,
 "The Quenching of Metastable O₂(¹Δ_g) and O₂(¹Σ_g⁺) Molecules,"
Chem. Phys. Letters 8, 259-62
- (71. 69) D. W. McCullough and W. D. McGrath,
 "The Collisional Deactivation of O(¹D) Atoms by Molecular Oxygen,"
Chem. Phys. Letters 8, 353-7
- (71. 70) D. R. Snelling and M. Gauthier,
 "Efficiency of O₂(¹Σ_g⁺) Formation by O(¹D) + O₂,"
Chem. Phys. Letters 9, 254-6
- (71. 71) S. Durmaz and J. N. Murrell,
 "The Effect of Rotations on the Predissociation Probabilities of
 Diatomic Molecular Spectra,"
Molec. Phys. 21, 209-16
- (71. 72) K. A. Dick and G. G. Sivjee,
 "O₂ Herzberg I Bands in the Night Airglow: Covariation With OI,"
J. Geo. Res. 76, 6987-9
- (72. 73) P. H. Krupenie,
 "The Spectrum of Molecular Oxygen,"
J. Phys. Chem. Ref. Data 1, 423-534
- (72. 74) U. Mingelgrin, R. G. Gordon, L. Frenkel, and T. E. Sullivan,
 "Microwave Spectrum of Compressed O₂-Foreign Gas Mixtures in
 the 48-41 GHz Region,"
J. Chem. Phys. 57, 2923-31
- (72. 75) K. Furukawa and E. A. Ogryzlo,
 "A Redetermination of the Rate Constants for the Quenching of
 Gaseous O₂(¹Δ_g) by Aliphatic Amines,"
J. Photochem. 1, 163-9
- (72. 76) D. W. McCullough and W. D. McGrath,
 "Electronic-Vibrational Energy Transfer in the Reaction of O(¹D)
 Atoms With Molecular Oxygen,"
J. Photochem. 1, 241-53
- (72. 77) S. D. Peyerimhoff and R. J. Buenker,
 "Comparison of Various CI Treatments for the Description of
 Potential Curves for the Lowest Three States of O₂,"
Chem. Phys. Letters 16, 235-43
- (72. 78) R. H. Pritchard, M. L. Sink, J. D. Allen, and C. W. Kern,
 "Theoretical Studies of Fine Structure in the Ground State of O₂,"
Chem. Phys. Letters 17, 157-9

- (72. 79) D. C. Cartwright, S. Trajmar, and W. Williams,
"The Excitation of O₂ in Auroras,"
Ann. Geophys. 28, 397-401
- (72. 80) H. C. Chang and M. Ogawa,
"Rotational Analysis of a High-Resolution Absorption Band of O₂
at 1161Å,"
J. Molec. Spectrosc. 44, 405-6
- (72. 81) A. Konkov and A. V. Vorontsov,
"Experimental Study of Infrared Radiation of Oxygen,"
Opt. Spectrosc. 32, 243-6
- (72. 82) P. B. Merkel and D. R. Kearns,
"Radiationless Decay of Singlet Molecular Oxygen in Solution. An
Experimental and Theoretical Study of Electronic-to-Vibrational
Energy Transfer,"
J. Am. Chem. Soc. 94, 7244-53
- (72. 83) P. Gerber,
"Hyperfine Structure From the Electron Spin Resonance Spectrum
of Gas Phase Oxygen,"
Helv. Phys. Acta 45, 655-82
- (72. 84) P. S. Julienne and M. Krauss,
"Excitation of O₂ ¹Δ_g by Electron Impact,"
J. Res. Nat. Bur. Stand. 76A, 661-3
- (72. 85) J. F. Noxon and A. E. Johanson,
"Changes in Thermospheric Molecular Oxygen Abundance Inferred
From Twilight 6300Å Airglow,"
Planet. Space Sci. 20, 2125-51
- (72. 86) J. H. Moore, Jr.,
"Electronic Excitation of N₂ and Dissociative Excitation of O₂ by
Proton Impact,"
J. Geo. Res. 77, 5567-72
- (72. 87) K. R. Yamawaki,
"Absorption Spectrum of O₂ in the a¹Δ_g Metastable State in the
Region From 1090 to 1700Å,"
Thesis, University of Southern California
- (73. 88) F. Koike and T. Watanabe,
"On the Mechanism of Electron Attachment by O₂,"
J. Phys. Soc. Japan 34, 1022-8

- (73. 89) F. Koike,
"Resonant Vibrational Excitation of O₂ by Slow Electron Impact,"
J. Phys. Soc. Japan 35, 1166-70
- (73. 90) G. R. Cook, M. Ogawa, and R. W. Carlson,
"Photodissociation Continuums of N₂ and O₂,"
J. Geo. Res. 78, 1663-7
- (73. 91) L. C. Lee, R. W. Carlson, D. L. Judge, and M. Ogawa,
"The Absorption Cross Sections of N₂, O₂, CO, NO, CO₂, N₂O,
CH₄, C₂H₄, C₂H₆ and C₄H₁₀ From 180 to 700 Å,"
J. Quant. Spectrosc. Rad. Trans. 13, 1023-31
- (73. 92) D. L. Albritton, W. J. Harrop, and A. L. Schmeltekopf,
"Calculation of Centrifugal Distortion Constants for Diatomic
Molecules From RKR Potentials,"
J. Molec. Spectrosc. 46, 25-36
- (73. 93) D. L. Albritton, W. J. Harrop, A. L. Schmeltekopf, and R. N. Zare,
"Resolution of the Discrepancies Concerning the Optical and Micro-
wave Values for B₀ and D₀ of the X³Σ_g⁻ State of O₂,"
J. Molec. Spectrosc. 46, 103-18
- (73. 94) M. Gauthier and D. R. Snelling,
"Possible Production of O₂(¹Δ_g) and O₂(¹Σ_g⁺) in the Reaction of NO
With O₃,"
Chem. Phys. Letters 20, 178-81
- (73. 95) C. Schmidt and H. I. Schiff,
"Reactions of O₂(¹Δ_g) With Atomic Nitrogen and Hydrogen,"
Chem. Phys. Letters 23, 339-42
- (73. 96) V. D. Galkin,
"Line Shifts in the A Oxygen Band as a Function of the Pressure,"
Opt. Spectrosc. 35, 630-3
- (73. 97) V. D. Galkin, L. N. Zhukova, and L. A. Mitrofanova,
"Line Intensities and Halfwidths in the A and B Bands of the Red
Atmospheric Band System of O₂,"
Opt. Spectrosc. 33, 462-5
- (73. 98) D. C. Cartwright, W. J. Hunt, W. Williams, S. Trajmar, and
W. A. Goddard III,
"Theoretical and Experimental (Electron-Impact) Studies of the
Low-Lying Rydberg States in O₂,"
Phys. Rev. A 8, 2436-48

- (73. 99) R. J. Collins and D. Husain,
"A Kinetic Study of Vibrationally Excited O₂(a¹Δ_g, v = 1) by Time-Resolved Absorption Spectroscopy in the Vacuum Ultra-Violet,"
J. Photochem. 1, 481-90
- (73. 100) W. S. Watson, J. Lang, and D. T. Stewart*,
"Photoabsorption Coefficients of Molecular Oxygen in the 400-600Å Region,"
Phys. Letters 44A, 293-4
- (73. 101) J. A. Kinsinger and J. W. Taylor,
"Autoionization and the Photoelectron Spectra of Oxygen,"
Int. J. Mass Spect. Ion Phys. 11, 461-74
- (73. 102) S. F. Wong, M. J. W. Boness, and G. J. Schulz,
"Vibrational Excitation of O₂ by Electron Impact Above 4 eV,"
Phys. Rev. Letters 31, 969-72
- (73. 103) R. J. Collins, D. Husain, and R. J. Donovan,
"Kinetic and Spectroscopic Studies of O₂(a¹Δ_g) by Time-Resolved Absorption Spectroscopy in the Vacuum Ultra-Violet,"
J. Chem. Soc. Faraday Trans. II 69, 145-57
- (73. 104) J. G. Parker and D. N. Ritke,
"Vibrational Relaxation Times of Oxygen in the Pressure Range 10-110 atm,"
J. Chem. Phys. 58, 314-23
- (73. 105) J. A. Hall,
"Comment on the Spin-Orbit Contribution to the Zero-Field Splitting of the Oxygen Molecule,"
J. Chem. Phys. 58, 410-2
- (73. 106) T. J. Cook, B. R. Zegarski, W. H. Breckenridge, and T. A. Miller,
"Gas Phase EPR of Vibrationally Excited O₂,"
J. Chem. Phys. 58, 1548-52
- (73. 107) T. C. Frankiewicz and R. S. Berry,
"Production of Metastable Singlet O₂ Photosensitized by NO₂,"
J. Chem. Phys. 58, 1787-95
- (73. 108) I. T. N. Jones and K. D. Bayes,
"Formation of O₂(a¹Δ_g) by Electronic Energy Transfer in Mixture of NO₂ and O₂,"
J. Chem. Phys. 59, 3119-24

- (73. 109) J. G. Parker and D. N. Ritke,
"Collisional Deactivation of Vibrationally Excited Singlet Molecular Oxygen,"
J. Chem. Phys. 59, 3713-22
- (73. 110) P. D. Burrow,
"Dissociative Attachment From the O₂(a¹Δ_g) State,"
J. Chem. Phys. 59, 4922-31
- (73. 111) C. Long and D. R. Kearns,
"Selection Rules for the Intermolecular Enhancement of Spin Forbidden Transitions in Molecular Oxygen,"
J. Chem. Phys. 59, 5729-36
- (74. 112) J. A. Davidson and E. A. Ogryzlo,
"The Quenching of O₂(¹Σ_g⁺) by Aliphatic Hydrocarbons,"
Can. J. Chem. 52, 240-5
- (74. 113) D. R. Snelling,
"The Ultraviolet Flash Photolysis of Ozone and the Reactions of O(¹D) and O₂(¹Σ_g⁺),"
Can. J. Chem. 52, 257-70
- (74. 114) C. M. Penney, R. L. St. Peters, and M. Lapp,
"Absolute Rotational Raman Cross Sections for N₂, O₂, and CO₂,"
J. Opt. Soc. Am. 64, 712-6
- (74. 115) D. L. Huestis, G. Black, S. A. Edelstein,
"Fluorescence and Quenching of O₂(¹Δ_g) and [O₂(¹Δ_g)]₂ in Liquid Oxygen,"
J. Chem. Phys. 60, 4471-4
- (74. 116) W. P. West, T. B. Cook, F. B. Dunning, R. D. Rundel, and R. F. Stebbings,
"Chemiiionization of O₂ Molecules by Helium Metastable Atoms,"
J. Chem. Phys. 60, 5126-7
- (74. 117) L. C. Lee, R. W. Carlson, D. L. Judge, and M. Ogawa,
"Vacuum Ultraviolet Fluorescence From Photodissociation Fragments of O₂ and N₂,"
J. Chem. Phys. 61, 3261-9
- (74. 118) J. G. Parker and D. N. Ritke,
"On the Mechanism for Collisional Deactivation of Vibrationally Excited Singlet Molecular Oxygen,"
J. Chem. Phys. 61, 3408-13

- (74. 119) L. Veseth and A. Lofthus,
"Fine Structure and Centrifugal Distortion in the Electronic and
Microwave Spectra of O₂ and SO,"
Molec. Phys. 27, 511-19
- (74. 120) L. P. Giver, R. W. Boese, and J. H. Miller,
"Intensity Measurements, Self-Broadening Coefficients, and
Rotational Intensity Distribution for Lines of the Oxygen B Band
at 6880 Å,"
J. Quant. Spectrosc. Rad. Trans. 14, 793-802
- (74. 121) E. A. Ogryzlo and B. A. Thrush,
"The Vibrational Excitation of H₂O and CO₂ by O₂(¹Σ_g⁺),"
Chem. Phys. Letters 24, 314-6
- (74. 122) T. J. Cook and T. A. Miller,
"Production of ¹Δ_g O₂ From Microwave Discharges in CO₂, NO₂
and SO₂,"
Chem. Phys. Letters 25, 396-8
- (74. 123) I. B. C. Matheson, J. Lee, B. S. Yamanashi, and M. L. Wolbarsht,
"Observation of the Singlet Oxygen Dimer Emission From Neodymium
Laser Pumped Oxygen in Gas Phase and in 1,1,2-Trichlorotrifluoro-
ethane Solution,"
Chem. Phys. Letters 27, 355-8
- (74. 124) L. E. Khvorostovskaya and V. A. Yankovskii,
"Mechanism of Ozone Formation in the Molecular Oxygen Glow
Discharge,"
Opt. Spectrosc. 37, 26-30
- (n. p. 125) D. L. Albritton, A. L. Schmeltekopf, and R. N. Zare,
"Diatomic Intensity Factors,"
(to be published by Harper and Row)

Methods of Production and Experimental Technique

Absorption in phosphorus vapor, flash photolysis of PH₃.

Emission from a discharge of He or H₂ with phosphorus, discharge in PH₃ or microwave discharge in PCl₃.

Fluorescence.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$A^1\Pi_g \leftarrow X^1\Sigma_g^+$	Emission	3110-2850	R	2970(0, 1)		(73.42, 58.21)
	II	$C^1\Sigma_u^+ \rightleftharpoons X^1\Sigma_g^+$	Emission	3500-2000	R	2953.6(6, 22) 2757.1(4, 17) 2456.9(3, 10)		(67.31, 67.30, 66.24, 64.23, 61.22, 50.18, 50.17, 49.16, 46.14, 43.12, 43.11, 40.10, 35.9, 33.8, 32.7, 32.6, 32.5, 32.4, 31.3, 30.2, 07.1)
			Absorption	2300-1800	R	2108.1(3, 1)		
	III	$E^1\Pi_u \rightleftharpoons X^1\Sigma_g^+$	Absorption, emission	1750-1600	R	1705.5(0, 1) 1728.1(0, 2)		(66.24, 55.20, 55.19)
	IV	$G^1\Sigma_u^+ \rightleftharpoons X^1\Sigma_g^+$	Absorption, emission	1530-1480	R	1508.7(0, 0)		(66.24, 55.19)
	V	$I^1\Pi_u \leftarrow X^1\Sigma_g^+$	Absorption	1480-1460	R	1460.7(0, 0)		(66.24)
	VI	$K^1\Pi_u \leftarrow X^1\Sigma_g^+$	Absorption	1400-1320	R	1384.0(0, 0)		(66.24)
	VII	$M^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$	Absorption	1350-1300	R	1355.1(0, 0)		(66.24)
	VIII	$N^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$	Absorption	1310-1290	R	1294.5(0, 0)		(66.24)

 Molecule P₂

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	IX	$Q^1\Pi_u \rightarrow X^1\Sigma_g^+$	Absorption	~ 1250	R	1253.5(0,0)		(66.24)
	X	$S^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$	Absorption	~ 1227	R	1227.6		(66.24)
	XI	$b^3\Sigma_u^- \rightarrow X^1\Sigma_g^+$	Emission	4400-3500	R	3720.1(0,2) 3828.8(0,3)		(74.44, 67.29)
	XII	$B^1\Pi_u \rightarrow A^1\Pi_g$	Emission	6674-6270		6414.0(0,0)		(72.42, 71.40)
	XIII	$c(^3\Pi_u) \rightarrow b(^3\Pi_g)$	Emission	10050-7700	V	8622.0(4,2) 8738.9(4,2) 8829.2(4,2)		(68.32, 67.29, 67.27, 64.23)

Molecule P₂

I. $A^1\Pi_g \rightarrow X^1\Sigma_g^+$ System

Band heads, λ (58.21):

(v', v'')	(0, 3)	(0, 2)	(0, 1)	(0, 0)	(1, 0)
λ	3112.43	3039.29	2969.84	2902.99	2852.23

II. $C^1\Sigma_u^+ \approx X^1\Sigma_g^+$ System

Band heads, λ

v', v''	0	1	2	3	4	5	6	7
0	2136.58				2286.36	2326.5	2367.6	2409.9
1	2115.23	2150.0	2186.4		2261.6	2301.0		
2	2094.38	2128.6		2164.3			2315.97	2356.3
3	2074.66	2108.1			2143.0	2253.24	2291.8	
4	2055.32	2088.3		2157.35		2122.6	2267.86	
5	2036.55	2069.0			2172.2		2245.4	2283.2
6	2018.08	2050.0					2223.0	
7	2000.26					2165.9		
8	1983.52					2145.31	2180.43	2216.1
9	1966.61		2027.52		2092.21		2159.89	2195.01
10	1950.15		2009.80			2073.56		

III. $E^1\Pi_u \approx X^1\Sigma_g^+$ System

Band heads, λ (66.24, 55.19):

v', v''	0	1	2	3	4
0	1683.22	1705.47	1728.14	1751.23	
1	1663.76		1709.6	1732.24	1755.10
2	1644.92				
3	1626.65				
4	1608.89				

P₂

IV. $G^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$ System

Band heads, λ (66.24, 55.19):

v', v''	0	1	2	3	4	5
0	1508.68	1526.50				
1	1493.30	1510.75	1528.45			
2	1478.39	1495.51	1512.85	1530.54		
3		1480.74	1497.77	1515.07		
4				1500.12	1517.33	
5					1502.53	1519.67
6						

V. $I^1\Pi_u \leftarrow X^1\Sigma_g^+$ System

Band heads, λ (66.24):

(v', v'')	(0, 1)	(0, 0)
λ	1477.42	1460.69

VI. $K^1\Pi_u \leftarrow X^1\Sigma_g^+$ System

Band heads, λ (66.24):

(v', v'')	(0, 1)	(0, 0)	(1, 0)	(2, 0)	(3, 0)	(4, 0)
λ	1398.98	1383.98	1370.67	1357.81	1345.17	1333.16

VII. $M^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$ System

Band heads, λ (66.24):

(v', v'')	(0, 0)	(1, 0)	(2, 0)	(3, 0)	(4, 0)
λ	1355.06	1342.82	1330.92	1319.33	1308.04

VIII. $N^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$ System

Band heads, λ (66.24):

(v, v'')	(1, 2)	(0, 1)	(2, 2)	(1, 1)	(0, 0)	(1, 0)	(2, 1)
λ	1309.82	1307.54	1299.96	1296.78	1294.47	1283.88	1287.09

IX. $Q^1\Pi_u \leftarrow X^1\Sigma_g^+$ System

Band heads, λ (66.24):

(v', v'') λ	(1, 1) 1255.94	(0, 0) 1253.45
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XI. $b'^3\Sigma_u^- \rightarrow X^1\Sigma_g^+$ System

Band heads, λ (74.44, 67.29):

v', v''	0	1	2	3	4
0		3617.9	3721.5	3830.4	3944.9
1		3541.0	3640.2		
2					3767.2

XII. $B^1\Pi_g \rightarrow A^1\Pi_u$ System

Band heads, λ (73.42):

(v', v'') λ	(0, 2) 6674.0	(1, 2) 6517.8	(0, 0) 6414.0	(1, 0) 6269.7
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XIII. $c(^3\Pi_u) \rightarrow b(^3\Pi_g)$ System

Band heads, λ (67.29, 67.27, 64.23):

v', v''	λ			v', v''	λ		
0, 0	10047.5	9934.7	9784.9	2, 0	8924.6	8829.2	8716.8
1, 0	9449.2	9345.8	9218.3	3, 1	8875.4	8786.5	8673.6
2, 1	9389.7	9289.5	9159.1	4, 2	8829.2	8738.9	8622.0
3, 2	9325.8	9218.3	9105.0	5, 3	8786.5	8693.3	8585.7
4, 3	9269.6	9159.2	9047.3	6, 4	8738.9	8648.1	8537.4

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e \omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$S^1\Sigma_u^+$	81843.6 ^(a)	-	-	0.2783 ^(d)	-	-	1.978 ^(e)		(66.24)
$Q^1\Pi_u$	80169.2 ^(a)	618 ^(b)	-	-	-	-	-		(66.24)
$N^1\Sigma_u^+$	77286.8	701.2	(29.70)	0.29845	5.11	3.1	1.910		(66.24)
$M^1\Sigma_u^+$	73845.7	678.5	3.0	0.2786	1.6	-	1.977		(66.24)
$K^1\Pi_u$	72288.5	713	5.5	0.2704 ^(d)	-	-	2.006 ^(e)		(66.24)
$I^1\Pi_u$	68849.4	-	-	0.2541 ^(d)	-	2.5	2.070 ^(e)		(66.24)
$G^1\Sigma_u^+$	66313.43	694.12	4.18	0.2973	1.95	2.25	1.913		(66.24, 55.19)
$E^1\Pi_u$	59446.28	700.66	2.92	0.2807 ^(d)	-	1.84	1.969 ^(e)		(66.24, 55.19)
$B^1\Pi_g$	50223.30	391.3	16.2	0.2300	6.0	3.3	2.176		(73.42)
$C^1\Sigma_u^+$	46941.33	473.93	2.340	0.24211	1.75	2.57	2.1204	(c)	(66.24)
$A^1\Pi_g$	34515.34	618.78	2.92	0.2752	1.70	2.2	1.9889		(73.42, 58.21)

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_{ee}\omega_e$	B_e	$\alpha_e \times 10^5$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$c(^3\Pi_u)$	10180 + x_1 10038 + x_2 9915 + x_3	640 (f)	4.0						(67.29)
$b'^3\Sigma_u^-$	28507.74	604.48	2.2	0.2583	1.4	1.6			(74.44, 73.43, 67.29)
$b(^3\Pi_g)$	x_1, x_2, x_3	562	3.6						(67.29)
$x^1\Sigma_g^+$	0	780.89	2.820	0.30356	1.43	1.88	1.8937	(g)	(73.43, 67.31, 66.24)

(a) $T_e + G'(0)$; (b) $\Delta G_{1/2}$; (c) $y_{ee}^w = 0.0066 \text{ cm}^{-1}$; (d) B_0 ; (e) r_0 ; (f) v uncertain;

(g) $y_{ee}^w = -0.005511 \text{ cm}^{-1}$

Dissociation energy = $5.04 \pm 0.11 \text{ eV}$, 147.5 kcal/mole , 40651 cm^{-1} (68.34).

Perturbations and General Information

Many of the vibrational levels of the $C^1\Sigma_u^+$ state are strongly perturbed (50.18, 50.17, 32.4).

Many of the levels of the $E^1\Pi_u$ state are perturbed (66.24).

Predissociation of the $C^1\Sigma_u^+$ state, by a $^3\Sigma_u^+$ state, is observed at $v = 10$, $J = 58$ and $v = 11$, $J = 34$. A second predissociation is observed at $v = 19$ (66.24).

A region of diffuse absorption at 1425\AA probably belongs to the I - X system.

Levels of the $K^1\Pi_u$ state are diffuse (maximum at $v = 3, 4$), probably due to predissociation.

Potential energy curves - RKR potentials (70.36):

State	v	$U+T_e(\text{cm}^{-1})$	$r_{\min}(\text{\AA})$	$r_{\max}(\text{\AA})$
$E^1\Pi_u$	0	59795.9	1.914	2.025
	1	60490.9	1.879	2.073
	2	61179.3	1.854	2.106
	3	61862.2	1.836	2.135
	4	62540.8	1.821	2.160
$G^1\Sigma_u^+$	0	66659.4	1.860	1.972
	1	67341.8	1.825	2.020
	2	68016.9	1.800	2.054
	3	68683.4	1.782	2.084
	4	69341.3	1.767	2.111
	5	69990.7	1.754	2.136
	6	70631.2	1.742	2.160
$K^1\Pi_u$	0	72643.6	1.966	2.076
	1	73345.3	1.932	2.125
	2	74036.0	1.911	2.161
	3	74728.1	1.895	2.193
	4	75398.1	1.864	2.194
	5	76078.2	1.857	2.232
$M^1\Sigma_u^+$	0	74184.2	1.922	2.035
	1	74856.4	1.886	2.083
	2	75523.5	1.862	2.118
	3	76182.5	1.842	2.146
	4	76836.6	1.828	2.173

State	v	U+T _e (cm ⁻¹)	r _{min} (Å)	r _{max} (Å)
N ¹ Σ _u ⁺	0	77286.8	1.858	1.972
	1	78264.0	1.828	2.032
	2	78844.0	1.805	2.079

BIBLIOGRAPHY

- (07. 1) Emission,
P. Geuter,
Z. Wiss. Phot. 5, 33-60
- (30. 2) Predissociation,
G. Herzberg,
Nature 126, 239-40
- (31. 3) Absorption and Fluorescence,
A. Jakovleva,
Z. Physik 69, 548-63
- (32. 4) Emission,
G. Herzberg,
Ann. Phys. 15, 677-706
- (32. 5) F. A. Jenkins and M. F. Ashley,
Nature 129, 829-30
- (32. 6) G. Herzberg,
Phys. Rev. 40, 313-4
- (32. 7) F. A. Jenkins and M. F. Ashley,
Phys. Rev. 39, 552
- (33. 8) Emission
M. F. Ashley,
Phys. Rev. 44, 919-26
- (35. 9) Nuclear Spin,
F. A. Jenkins,
Phys. Rev. 47, 783
- (40. 10) Absorption,
G. Herzberg, L. Herzberg, and G. G. Milne,
Can. J. Res. 18, 139-43
- (43. 11) Emission,
K. N. Rao,
Indian J. Phys. 17, 135-40
- (43. 12) Nuclear Spin,
K. N. Rao,
Indian J. Phys. 17, 149-52

- (44. 13) R. F. Barrow,
Proc. Phys. Soc. 56, 211-2
- (46. 14) Emission,
E. J. Marais,
Phys. Rev. 70, 499-510
- (48. 15) Emission,
K. Sreeramamurty,
Current Sci. 17, 119-20
- (49. 16) L. Gerö and C. Fonô,
J. Chem. Phys. 17, 345-6
- (50. 17) Emission,
E. J. Marais and H. Verleger,
Phys. Rev. 80, 429-31
- (50. 18) Perturbations,
S. M. Naude and H. Verleger,
Phys. Rev. 80, 432-5
- (55. 19) Emission,
K. Dressler,
Helv. Phys. Acta 28, 563-90
- (55. 20) K. Dressler and E. Miescher,
Proc. Phys. Soc. 68, 542-4
- (58. 21) Emission,
A. E. Douglas and K. S. Rao,
Can. J. Phys. 36, 565-70
- (61. 22) Flash Photolysis,
R. W. G. Norrish and G. A. Oldershaw,
Proc. Roy. Soc. 262, 1-9
- (64. 23) Emission,
H. Guenebaut, B. Pascat, and J. Brion,
C. R. Acad. Sci. 259, 3545-8
- (66. 24) Absorption,
F. Creutzberg,
Can. J. Phys. 44, 1583-92
- (66. 25) Dissociation Energy,
K. A. Gingerich,
J. Chem. Phys. 44, 1717-18

- (66. 26) R. B. Singh and D. K. Rai,
"Potential Curves for Some Diatomic Molecules: P₂, PN, SiN, NBr,
BaO, BeF, SiF and SnF,"
Indian J. Pure Appl. Phys. 4, 102-5
- (67. 27) Emission,
J. Brion, J. Malicet, and H. Guenebaut,
C. R. Acad. Sci. 264, 622-5
- (67. 28) Theory,
D. B. Boyd and W. N. Lipscomb,
J. Chem. Phys. 46, 910-9
- (67. 29) Emission,
A. Weber, S. P. S. Porto, L. E. Cheesman, and J. J. Barrett,
J. Opt. Soc. Am. 57, 19-28
- (67. 30) Flash Photolysis,
N. Basco and K. K. Yee,
Nature 216, 998-9
- (67. 31) Emission,
M. N. Dixit,
Proc. Indian Acad. Sci. A 66, 325-41
- (68. 32) Emission,
J. Brion, J. Malicet, and H. Guenebaut,
C. R. Acad. Sci. 266, 82-3
- (68. 33) F. Jenč,
"Ground State Reduced Potential Curves (RPC) of BeF, CS, SiN, P₂,
SiS and GeO,"
Spectrochimica Acta 24A, 259-64
- (68. 34) K. A. Gingerich,
"Gaseous Phosphorus Compounds. III. Mass Spectrometric Study
of the Reaction Between Diatomic Nitrogen and Phosphorus Vapor
and Dissociation Energy of Phosphorus Mononitride and Diatomic
Phosphorus,"
J. Phys. Chem. 73, 2734-41
- (69. 35) G. A. Ozin,
"Gas-Phase Raman Spectroscopy of Phosphorus, Arsenic, and
Saturated Sulphur Vapours,"
J. Chem. Soc. D 1969, 1325-7

- (70.36) T. V. R. Rao and S. V. J. Lakshman,
 "Potential Energy Curves, r-Centroids and Franck-Condon Factors
 for the Bands of P₂ Molecule,"
Indian J. Pure Appl. Phys. 8, 617-20
- (70.37) I. R. Beattie, G. A. Ozin, and R. O. Perry,
 "The Gas-Phase Raman Spectra of P₄, P₂, As₄, and As₂. The
 Resonance Fluorescence Spectrum of ⁸⁰Se₂. Resonance Fluorescence-
 Raman Effects in the Gas-Phase Spectra of Sulphur and I₂. The Effect
 of Pressure on the Depolarization Ratios for I₂,"
J. Chem. Soc. A 12, 2071-4
- (70.38) R. D. Verma and H. P. Broida,
 "Spectral Study of the Phosphorus Glow,"
Can. J. Phys. 48, 2991-5
- (71.39) B. Rai, J. Singh, and D. K. Rai,
 "Dissociation Energies of S₂, SO, Te₂, SeO and P₂,"
Israel J. Chem. 9, 563-8
- (71.40) J. Brion, J. Malicet, and J. Mongin,
 "Rotational Analysis of Two Bands of the New Visible Electronic
 System of the P₂ Radical,"
C. R. Acad. Sci. B 272, 127-30
- (73.41) J. Kordis and K. A. Gingerich,
 "Mass Spectroscopic Investigation of the Equilibrium Dissociation of
 Gaseous Sb₂, Sb₃, Sb₄, Sb₅, SbP₃ and P₂,"
J. Chem. Phys. 58, 5141-9
- (73.42) J. Malicet, J. Brion, and H. Guenebaut,
 "Analysis of Four Bands From a New ¹Π - ¹Π Transition of the P₂
 Radical,"
C. R. Acad. Sci. C 276, 991-4
- (73.43) J. Brion and J. Malicet,
 "Rotational Analysis of the (1, 1) Band of the a ³Σ_u⁻ - X ¹Σ_g⁺ Transition
 in the P₂ Radical,"
C. R. Acad. Sci. C 278, 223-6
- (74.44) J. Brion, J. Malicet, and H. Guenebaut,
 "Emission Spectra of the P₂ Radical: Study of the b' ³Σ_u⁻ - X ¹Σ_g⁺
 Transition,"
Can. J. Phys. 52, 2143-4

Pb₂

Pb₂

Methods of Production and Experimental Technique

Absorption.

Thermal emission.

Laser-induced fluorescence.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	A \rightarrow X	Absorption, fluorescence	7000-6200	R			(72.9, 67.8)
	II	B \rightarrow X	Absorption, fluorescence	5270-4200	R			(72.9, 67.8, 35.4)
	III	C \rightarrow X	Absorption	3000-2830	R			(n.p. 10, 67.8)
	IV	D \rightarrow X	Absorption	2780-2620	R			(n.p. 10, 67.8)
	V	E \rightarrow X	Absorption	2600-2460				(n.p. 10)
	VI	F \rightarrow X	Absorption	2450-2300	R			(n.p. 10, 67.8)
	VII	G \rightarrow X	Absorption	2167-2136				(n.p. 10)

Molecule Pb₂

II. B \leftarrow X SystemBand heads, λ (72.9):

(v', v'')	(3, 2)	(3, 1)	(3, 0)	(4, 1)	(4, 0)	(5, 0)
λ	5058.30	5030.56	5002.95	4991.79	4964.50	4927.56

III. C \leftarrow X SystemMost intense band heads, λ (n.p. 10):

λ	3003.1	2942.3	2931.3	2920.4	2911.0	2901.0
Intensity	10	4	5	6	7	7

V. E \leftarrow X System

Most intense ultraviolet system, with several bands converging (n.p. 10).

VI. F \leftarrow X SystemMost intense band heads, λ (Intensity) (n.p. 10):

λ	2435.7	2430.4	2417.4	2410.1	2403.4	2397.0	2390.7
Intensity	9	10	7	6	6	5	5

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e \omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
B	19490.3	161.64	1.036					(a)	(72.9)
A	14465.5	162.4	0.4						(72.9)
X	0	119.1	0.35						(72.9)
(a) $y_e \omega_e = 0.0055 \text{ cm}^{-1}$ Dissociation energy = $0.8 \pm 0.2 \text{ eV}$, 18.5 kcal/mole , 6450 cm^{-1}									

BIBLIOGRAPHY

- (32. 1) Attributed to Pb₂, possibly PbS,
 M. Domariewska-Kruger,
 Acta Phys. Polon. 1, 357-62
- (33. 2) Attributed to Pb₂, possibly PbS,
 W. Kloskowska,
 Acta Phys. Polon. 2, 239-44
- (35. 3) Ultraviolet, Low Resolution,
 N. V. Kremenevskii,
 C. R. Acad. Sci. (USSR) 3, 251-2
- (35. 4) Absorption and Emission,
 E. N. Shawhan,
 Phys. Rev. 48, 343-6
- (39. 5) Attributed to Pb₂, possibly N₂,
 L. Natanson,
 Acta Phys. Polon. 7, 275-8
- (57. 6) Dissociation Energy,
 J. Drowart and R. E. Honig,
 J. Phys. Chem. 61, 980-5
- (62. 7) Absorption,
 J. G. Kay, N. A. Kuebler, and L. S. Nelson,
 Nature 194, 671
- (67. 8) Absorption, Vibrational Analysis,
 S. Weniger,
 J. Phys. 28, 595-601
- (72. 9) S. E. Johnson, D. Cannell, J. Lunacek, and H. P. Broida,
 "New Molecular Constants for the Ground Electronic State of Pb₂,"
 J. Chem. Phys. 56, 5723-5
- (n.p. 10) Ultraviolet Systems,
 B. Eisler and R. F. Barrow,
 Unpublished

Pd₂

Pd₂

Spectroscopic Constants

Dissociation energy = 1.13 ± 0.21 eV, 26 kcal/mole, 9114 cm^{-1} (69.3).

BIBLIOGRAPHY

- (62. 1) Dissociation Energy,
M. Ackerman, F. E. Stafford, and G. Verhaegen,
J. Chem. Phys. 36, 1560-2
- (67. 2) Observation,
K. A. Gingerich,
Naturwissenschaften 54, 43
- (69. 3) S. Lin, B. Strauss, and A. Kant,
"Dissociation Energy of Pd₂,"
J. Chem. Phys. 51, 2282-3

Po₂

Po₂

Methods of Production and Experimental Technique

Emission from an electrodeless discharge.

Band Systems

Emission, degrading R, has been observed in the region 5130-3600Å.

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e \omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
(0_u^+)	25149.3	108.532	0.4417						
$X(0_g^+)$	0	155.715	0.3353					(a)	
(a) $y_e \omega_e = -0.0003226 \text{ cm}^{-1}$ Dissociation energy = $1.89 \pm 0.1 \text{ eV}$, 43.5 kcal/mole , 15244 cm^{-1} .									

BIBLIOGRAPHY

- (57. 1) Vibrational Analysis,
G. W. Charles, D. J. Hunt, G. Pish, and D. L. Timma,
J. Opt. Soc. Am. 47, 291-7

Pr₂

Pr₂

Spectroscopic Constants

Dissociation energy = 1.30 ± 0.30 eV, 30 kcal/mole, 10490 cm^{-1} (72.1).

BIBLIOGRAPHY

- (72. 1) A. Kant and S. Lin,
"Dissociation Energies of the Homonuclear Diatomic Molecules of
the Rare Earths,"
Monatshefte für Chemie 103, 757-63

Rb₂Methods of Production and Experimental Technique

Absorption.

Emission from a discharge in Rb vapor, from a discharge in a heat pipe.

Laser-induced fluorescence.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$A^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$	Absorption, discharge	11000-8400	R	Max. ~ 10500		(71.20, 34.8)
	II	$B^1\Pi_u \rightarrow X^1\Sigma_g^+$	Absorption, discharge	7350-6400	R	6824.2(1,1) 6797.8(1,0)		(71.20, 36.10)
	III	$C^1\Pi_u \rightarrow X^1\Sigma_g^+$	Absorption, laser-induced fluorescence	5030-4690	R	4746.5(10,2)		(71.20, 37.11)
	IV	$D \rightarrow X^1\Sigma_g^+$	Absorption	4550-4220	R	4326.8(10,1) 4288.2(14,0)		(37.11)
	V	$? \rightarrow X^1\Sigma_g^+$	Laser-induced fluorescence	6100-5400			Quasi-continuum	(71.20)
	VI	Bands associated with resonance lines (Van der Waals molecules)						(35.7, 32.6)

Molecule Rb₂

Rb₂

I. A¹Σ_u⁺ ≈ X¹Σ_g⁺ System

Bands are fragmentary, not analyzed (71.20, 34.8):

λ | 10500 | 9033 | 8989 | 8941 | 8897 | 8852 | 8807 | 8762

II. B¹Π_u ≈ X¹Σ_g⁺ System

Band heads of ⁸⁵Rb₂ of greatest intensity, λ (Intensity) (36.10):

(v', v'')	(1, 0)	(2, 0)	(3, 0)	(4, 0)	(6, 1)	(5, 0)
λ	6797.8	6775.7	6754.5	6734.0	6718.1	6713.2
(Intensity)	10	10	10	10	5	6

III. C¹Π_u ≈ X¹Σ_g⁺ System

Band heads of greatest intensity, λ (Intensity) (71.20, 37.11):

(v', v'')	(2, 1)	(3, 0)	(4, 0)	(6, 1)	(9, 2)	(8, 1)	(10, 2)
λ	4797.1	4775.8	4767.7	4764.6	4754.1	4749.0	4746.5
(Intensity)	9	8	8	8	8	9	10

IV. D - X¹Σ_g⁺ System

Band heads of greatest intensity, λ (Intensity) (37.11):

(v', v'')	(7, 2)	(8, 2)	(8, 1)	(9, 1)	(10, 1)	(11, 1)	(11, 0)
λ	4359.3	4351.9	4341.1	4333.8	4326.8	4319.7	4309.2
(Intensity)	8	8	9	9	10	9	9

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e \omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
D	22777.5	40.42	0.745					(e)	(37.11)
$C^1\Pi_u$	20835.1	36.46	0.124						(37.11)
$B^1\Pi_u$	14662.1	^(a) 48.05	^(c) 0.191						(36.10)
$A^1\Sigma_u^+$	~ 11500	-	-						(34.8)
$X^1\Sigma_g^+$	0	^(b) 57.31	^(d) 0.105	~ 0.02					(71.20, 37.11, 36.10)
<p>(a) $\omega_e = 47.78$ for $^{85}\text{Rb}^{87}\text{Rb}$, (b) $\omega_e = 56.98$ for $^{85}\text{Rb}^{87}\text{Rb}$, (c) $x_e \omega_e = 9.188$ for $^{85}\text{Rb}^{87}\text{Rb}$, (d) $x_e \omega_e = 0.103$ for $^{85}\text{Rb}^{87}\text{Rb}$, (e) $y_e \omega_e = -0.00144$ Dissociation energy = 0.47 ± 0.05 eV, 10.8 kcal/mole, 3790 cm^{-1}.</p>									

Molecule Rb_2

Rb₂

Perturbations and General Information

Radiation in the region 6100-5400 Å due to transfer from the C state into an unidentified state followed by transitions to high-lying and continuum levels of the ground state (71.20).

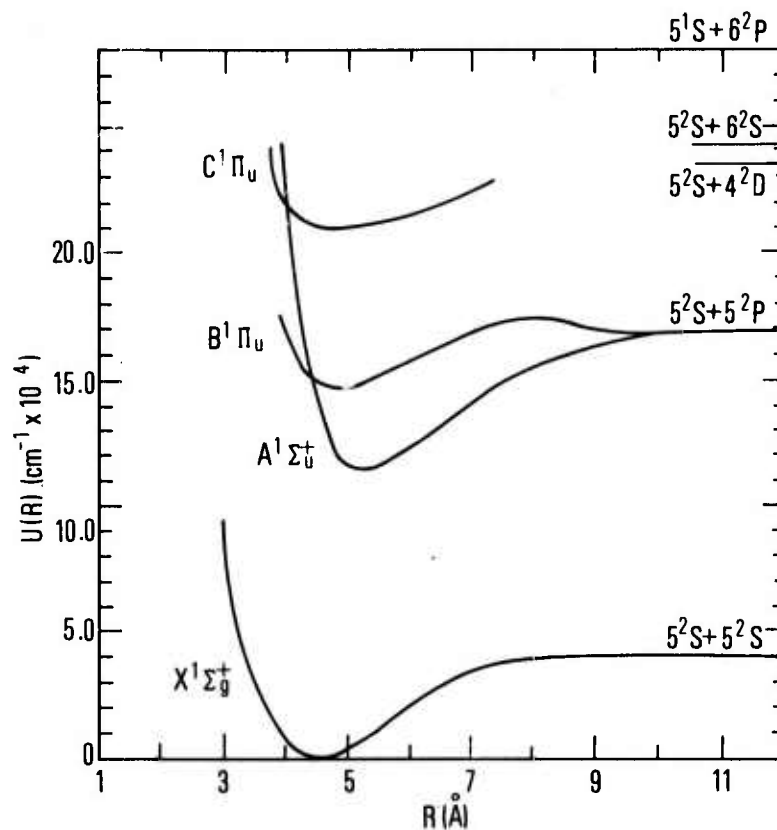
Predissociation of the C state caused by crossing of A state (71.20).

Radiative lifetimes (70.17):

$$B^1\Pi_u - \tau_r \sim 16 \text{ nsec}$$

$$C^1\Pi_u - \tau_r \sim 61 \text{ nsec}$$

Potential energy curves - empirical (71.20)



Average electric dipole polarizability (534°K) $68 \pm 7 \times 10^{-24} \text{ cm}^3$ (74.25).

BIBLIOGRAPHY

- (10. 1) Low Dispersion Investigation,
T. S. Carter,
Z. Physik 11, 632-3
- (11. 2) Low Dispersion Investigation,
P. V. Bevan,
Proc. Roy. Soc. A 85, 58-76
- (12. 3) Low Dispersion Investigation,
L. Dunager,
Radium 99, 218-23
- (23. 4) Low Dispersion Investigation,
J. C. MacLennan and D. S. Ainslie,
Proc. Roy. Soc. A 103, 304-14
- (28. 5) Low Dispersion Investigation,
J. M. Walter and S. Barratt,
Proc. Roy. Soc. A 119, 257-75
- (32. 6) Bands Associated With Resonance Lines,
S. Datta and B. Chakravarty,
Indian J. Phys. 7, 273-82
- (34. 7) E. Matuyama,
Nature 133, 567-8
- (34. 8) D \leftarrow X System, Incorrect Analysis,
E. Matuyama,
Sci. Rep. Tohoku Univ. 23, 296-307
- (35. 9) Bands Associated With Resonance Lines,
N. Tsi-Ze and C. Shin-Piaw,
J. Phys. Radium 6, 203-8
- (36. 10) B \rightleftharpoons X System,
P. Kusch,
Phys. Rev. 49, 218-22
- (37. 11) C, D \leftarrow X Systems,
H. Yoshimaga,
Proc. Phys. -Math. Soc. 19, 847-59

- (37. 12) Comparative Tables,
C. H. D. Clark,
Trans. Faraday Soc. 33, 1390-4
- (37. 13) Comparative Tables,
C. H. D. Clark,
Trans. Faraday Soc. 33, 1398-401
- (37. 14) Comparative Tables,
C. H. D. Clark and C. W. Scaife,
Trans. Faraday Soc. 33, 1394-8
- (40. 15) Comparative Tables,
R. F. Barrow,
Trans. Faraday Soc. 36, 624-5
- (68. 16) D. M. Creek and G. V. Marr,
"Some Ultraviolet Cross-Section Measurements on Molecular
Alkali-Metal Vapours,"
J. Quant. Spectrosc. Radiative Trans. 8, 1431-6
- (70. 17) G. Baumgartner, W. Demtröder, and M. Stock,
"Lifetime-Measurements of Alkali-Molecules Excited by Different
Laserlines,"
Z. Physik 232 462-72
- (71. 18) R. J. Gordon, Y. T. Lee, and D. R. Herschbach,
"Supersonic Molecular Beams of Alkali Dimers,"
J. Chem. Phys. 54, 2393-409
- (71. 19) Y. T. Lee, R. J. Gordon, and D. R. Herschbach,
"Molecular Beam Kinetics: Reactions of H and D atoms With
Diatomic Alkali Molecules,"
J. Chem. Phys. 54, 2410-23
- (71. 20) P. P. Sorokin and J. R. Lankard,
"Emission Spectra of Alkali-Metal Molecules Observed With a
Heat-Pipe Discharge Tube,"
J. Chem. Phys. 55, 3810-3
- (73. 21) N. N. Kostin, V. A. Khodovoy, V. V. Khromov, and N. A. Chigir,
"Optical Pumping and Dissociation of the Rb₂ Molecule by a Pulse
Laser,"
Zh. Eksp. Teor. Fiz. 14, 589-92
- (73. 22) N. N. Kostin and V. A. Khodovoy,
"Information on the Molecular Band Absorption of Rb₂ and Cs₂
Using Pulse Laser Radiation,"
Izvest. Akcad. Nauk 37, 2083-8

- (74.23) R. C. Oldenborg, J. L. Gole, and R. N. Zare,
"Chemiluminescent Spectra of Alkali-Halogen Reactions,"
J. Chem. Phys. 60, 4032-42
- (74.24) J. M. Brom, Jr. and H. P. Broida,
"Laser Photoluminescence and Photopredissociation of Rb₂,"
J. Chem. Phys. 61, 982-7
- (74.25) R. W. Molof, T. M. Miller, H. L. Schwartz, B. Bederson, and
J. T. Park,
"Measurements of the Average Electric Dipole Polarizabilities of
the Alkali Dimers,"
J. Chem. Phys. 61, 1816-22

Methods of Production and Experimental Technique

Absorption: at elevated temperatures, in matrices, after flash photolysis.

Emission: high frequency discharge, microwave discharge, flames.

Fluorescence: excited by OH*, laser-induced.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography
	I	$b^1\Sigma_g^+ \rightarrow X^3\Sigma_g^-$	Photolysis	11055-10920			Observation doubtful	(72.110)
	II	$B^3\Sigma_u^- \leftarrow X^3\Sigma_g^-$	Absorption, discharge, fluorescence	7110-2400	R	31589	(a)	(72.104, 68.90, 63.73, 62.69, 60.67, 53.61, 48.54)
	III	$C^3\Sigma_u^- \leftarrow X^3\Sigma_g^-$	Absorption	1870-1650	V	55633.3		(65.83, 48.56, 48.55, 34.26)
	IV	$C'^3\Sigma_u^- \leftarrow X^3\Sigma_g^-$	Microwave	1860-1760	V	56983.6	(b)	(62.71)
	V	$D^3\Pi_u \leftarrow X^3\Sigma_g^-$	Absorption	1750-1650	V	58750	(b)	(65.83, 48.55, 34.26)
	VI	$B'^3\Pi_{g,i} \leftarrow A^3\Sigma_u^+$	Discharge, microwaves	8083-7434	V	13447.7	(c)	(66.86, 64.76, 62.69, 35.28)
	VII	$B'^3\Pi_{g,i} \leftarrow A'^3\Sigma_{u,i}$	Discharge, microwaves	7761-6984	V	$^3\Pi_1 - ^3\Delta_2$ -14144.7 $^3\Pi_2 - ^3\Delta_3$ -14318.0	(c)	(64.76, 62.69, 35.28)
	VIII	$f^1\Delta_g \leftarrow a^1\Delta_g$	Absorption, discharge	3350-2400	R	36743		(70.103, 69.100, 64.78, 64.77, 64.76, 63.75)

Molecule S₂

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography
	IX	$g^1\Delta_u \rightarrow a^1\Delta_g$	Discharge, microwaves	2130-1880	V	52244.7		(68.93, 62.71)
	X	$h^1\Sigma_u^+ \rightarrow b^1\Sigma_g^+$	Discharge, microwaves	2130-1760	V	51401.3	(b)	(68.93, 67.89, 65.83, 62.71)
	XI	$i \rightarrow b^1\Sigma_g^+$	Discharge, microwaves	2130-1760	V	55448.3	(b)	(68.93, 65.83, 62.71)
	XII	$e^1\Pi_g \rightarrow c^1\Sigma_u$	Discharge	7430-7152	V	13452		(62.69)
	XIII	?	Microwaves	1850-1780	V	56077.7	(b)	(67.89)
<p>(a) Numerous perturbations and predissociations. Several bands possess secondary heads.</p> <p>(b) Analysis is uncertain.</p> <p>(c) Predissociates.</p>								

Molecule S₂

I. $b^1\Sigma_g^+ \rightarrow X^3\Sigma_g^-$ System

Observed in laser emission only (75.L117. 72.110).

λ | 11055 | 10975 | 10920

II. $B^3\Sigma_u^- \leftarrow X^3\Sigma_g^-$ System

Band heads of $^{32}\text{S}_2$, λ (Intensity) (36.30, 31.22, 31.21):

v', v''	0	1	2	3	4	5	6
0				3387.0(1)	3469.6(2)	3555.8(3)	3645.2(5) ^a
1			3259.9(2)	3336.7(2)	3417.0(4)	3500.5(5)	3587.4(5)
2		3143.7(1)	3216.1(2)	3290.7(3)	3369.6(4)	3451.0(2)	
3	3033.1(1)	3101.5(1)	3171.5(2)	3244.7(3)	3321.2(1)		
4	2997.0(1)	3063.6(3)	3132.4(3)	3203.2(2)			
5	2960.1(2)	3024.3(4)	3091.7(5)	3161.1(1)			
6	2926.6(2)	2989.7(4) ^a	3054.9(3)				

^a Bands possessing weak secondary heads

Isotope studies of $^{34}\text{S}_2$ (70.105).

III. $C^3\Sigma_u^- \leftarrow X^3\Sigma_g^-$ System

Each band possesses from 3 to 6 heads, with a maximum separation between extremes of 1 - 8Å. Isotope effect has been noted for several bands.

Most intense band heads, λ (Intensity) (65.83, 48.55):

v', v''	0	1	2	3	4	5
0	1796.93(9)	1820.46(4)	1844.43(3)	1868.82(1)	1894.50(1)	1919.81(1)
1	1770.75(9)		1816.88(1)	1840.51(1)	1864.65(1)	1889.93(1)
2	1745.57(8)	1768.99(2)				
3	1721.29(5)	1742.89(3)				
4	1697.97(4)	1718.90(2)				
5	1675.39(1)	1695.78(2)	1716.56(1)			
6	1653.60(1)	1673.52(1)	1693.72(1)			

S₂

IV. C'³Σ_u⁻ → X³Σ_g⁻ System

Double-headed bands with separation of ~ 14 cm⁻¹ are observed.
Most intense band heads, λ (Intensity) (62.71):

(v', v'')	(0, 4)	(0, 3)	(0, 2)	(0, 1)	(0, 0)
λ	1859.49	1835.57	1811.94	1788.84	1766.11
(Intensity)	1	2	2	5	4

V. D³Π_u ← X³Σ_g⁻ System

Each band has 9 heads. Most intense band heads of the a₃, b₃, and c₃ series, λ (Intensity) (65.83, 48.55):

v', v''	0	1	2	3	4
0 { a ₃	1709.95(10)	1729.18(1)	1750.93(1)		
0 { b ₃	1702.37(8)	1723.44(1)			
0 { c ₃	1694.60(10)	1715.83(1)	1737.02(0)		
1 { a ₃	1685.32(4)	1705.99(3)	1726.99(0)		
1 { b ₃	1679.88(4)	1700.49(3)			
1 { c ₃	1672.34(6)	1692.75(4)	1714.44(0)		
2 { a ₃	1663.49(2)	1683.63(2)	1704.08(1)	1724.91(0)	
2 { b ₃	1658.23(2)	1678.25(2)	1698.63(0)		
2 { c ₃	1650.85(2)	1670.87(6)		1711.34(0)	
3 { a ₃		1662.08(1)	1681.99(1)		
3 { b ₃		1656.85(0)	1676.65(1)		1717.19(0)
3 { c ₃		1649.49(1)	1669.16(1)		1709.36(0)

VI. $B'^3\Pi_{g,i} \rightarrow A'^3\Sigma_u^+$ System

Two subsystems - because the $^3\Pi_0$ state is completely predissociated. Only 5 of the 9 possible heads are observed (65.83). Isotope shifts (66.86).

Most intense band heads, λ (66.86, 64.76):

$$B'^3\Pi_2 \rightarrow A'^3\Sigma_u^+; (v', v'') \lambda | (0, 1) 7785.6 | (0, 0) 7506.8$$

$$B'^3\Pi_1 \rightarrow A'^3\Sigma_u^+; (v', v'') \lambda | (0, 1) 7707.4 |$$

VII. $B'^3\Pi_{g,i} \rightarrow A'^3\Delta_{u,i}$ System

Two subsystems - because the $^3\Pi_0$ state is completely predissociated. λ (64.76, 62.69):

$$B'^3\Pi_2 \rightarrow A'^3\Delta_{u,i}; (v', v'') \lambda | (0, 2) 7583 | (0, 1) 7328 | (0, 0) 7068$$

$$B'^3\Pi_1 \rightarrow A'^3\Delta_{u,i}; (v', v'') \lambda | (0, 3) 7759 | (0, 2) 7485 | (0, 1) 7228 | (0, 0) 6984$$

VIII. $f^1\Delta_u \approx a^1\Delta_g$ System

Single-headed bands. Isotope studies (65.82, 65.80).

Most intense band heads, λ (70.103, 64.77)

v', v''	0	1	2	3	4	5	6
0					2940.49	2999.74	3060.77
1				2847.52	2903.53		
2			2760.14	2813.24			
3		2677.92	2728.33				
4		2648.34	2697.64				
5		2619.78	2668.02				
6	2546.28	2592.52					
7	2520.56	2565.59					
8	2495.77						
9	2471.77						
10	2448.98						

IX. $g^1\Delta_u \rightarrow a^1\Delta_g$ System

Single-headed bands. Most intense band heads, λ (Intensity) (68.90, 62.71):

v', v''	0	1	2	3	4	5	6	7
0	1914.06 (9)	1939.89 (9)	1966.08 (9)	1992.63 (7)	2019.68 (6)	2047.24 (4)	2075.24 (3)	2103.73 (2)
1	1884.80 (6)		1934.96 (0)	1960.85 (3)	1987.12 (3)	2013.79 (4)	2040.90 (3)	2068.49 (2)
2			1905.09 (2)			1981.57 (2)	2007.91 (2)	2034.59 (1)
3							1976.15 (0)	2002.01 (1)

X. $h^1\Sigma_u^+ \rightarrow b^1\Sigma_g^+$ System

Most intense band heads, λ (Intensity) (68.90, 67.89, 65.83):

v', v''	0	1	2	3	4	5	6	7
0	1943.25 (4)	1969.75 (5)	1996.80 (5)	2024.18 (5)	2052.04 (3)	2080.47 (2)		
1				1991.44 (9)	2018.27 (4)	2045.87 (4)	2073.77 (3)	
2			1934.20 (5)		1985.95 (1)	2012.44 (3)	2039.66 (3)	2067.19 (2)
3			1905.09 (2)	1929.42 (1)			2006.75 (1)	2033.33 (1)

XI. $i \rightarrow b^1\Sigma_g^+$ System

Only a single head is observed. Most intense band heads, λ (Intensity) (68.93, 65.83, 62.71):

(v', v'')	(0, 7)	(1, 8)	(0, 6)	(1, 7)	(0, 5)
λ	1984.52	1979.18	1959.15	1954.07	1934.20
(Intensity)	3	2	0	2	5
(v', v'')	(1, 6)	(0, 4)	(1, 5)	(0, 2)	(1, 1)
λ	1929.44	1909.57	1905.09	1861.73	1811.94
(Intensity)	1	1	2	0	2

SPECTROSCOPIC CONSTANTS

State	T_0 (Observed)	T_0 (Calculated)	ω_e	$x_e \omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^8$	r_e	Remarks	Bibliography
$i^1\Sigma_u^+ 1\Delta_u$	$\begin{Bmatrix} 55448 + b \\ 55448 + a \end{Bmatrix}$	$\begin{Bmatrix} \sim 64000? \\ \sim 59900? \end{Bmatrix}$	-	-	>0.29	-	-	<1.9		(68.93, 65.83, 62.71)
$h^1\Sigma_u^+$	51401.3+b	$\sim 59900?$	819.6	2.70	>0.29	-	~ 14.52	<1.89		(65.83, 62.71)
$D^3\Pi_u$	58750	58750	793.9	4.0	0.3066	-	~ 16.293	(1.854)	(a)	(69.100, 65.83, 48.55)
$C'^3\Sigma_u^-$	56983.6	56984	-	-	>0.295	-	-	<1.89		(65.83)
$g^1\Delta_u$	52244.7+a	~ 56700	816.4	2.7	0.3217	1.44	20.0	1.811		(68.83)
$C^3\Sigma_u^-$	55633.3	55633.3	829.15	3.34	0.32196	1.4	22.0	1.810	(b)	(69.99, 65.83, 48.55)
$f^1\Delta_u$	36743.5+a	~ 41200	438.32	2.70	0.22704	1.78	24.5	2.155	(d)	(70.103, 68.93, 65.83)
$e^1\Pi_g$	13451.8+a	~ 37000	$\begin{matrix} (c) \\ 533.7 \end{matrix}$	-	~ 0.25	-	-	~ 2.08		(65.83)
$B'^3\Pi_{g,i}$	14144.7+A'	~ 36000	-	-	0.244	-	-	2.08	(e)	(65.83, 62.69)
$B^3\Sigma_u^-$	31689	31689	434	2.75	0.2244	1.8	23.1	2.168		(63.73)
$B''^3\Pi_u$	≤ 31700	≤ 31700	-	-	>0.2029	-	-	<2.280		(65.83, 63.73)
$A^3\Sigma_u^+$	697 + A'	~ 22550	$\begin{matrix} (c) \\ 477 \end{matrix}$	-	-	-	-	-		(65.83, 62.69)
$c^1\Sigma_u^-$	c	~ 23550	$\begin{matrix} (c) \\ 533.6 \end{matrix}$	-	~ 0.235	-	-	2.122		(62.69)
$A'^3\Delta_{u,i}$	A'	~ 21855	488.6	2.63	0.2284	1.40	19.96	2.148	(f)	(62.69)

Molecule S_2

SPECTROSCOPIC CONSTANTS

State	T _o (Observed)	T _o (Calculated)	ω_e	$x_e \omega_e$	B _e	$\alpha_e \times 10^3$	D _e × 10 ⁸	r _e	Remarks	Bibliography
b ¹ Σ _g ⁺	b	~ 8500	700.8?	3.4?	-	-	-	-		(65.83)
a ¹ Δ _g	a	~ 4500	702.35	3.09	0.29262	1.73	20.4	1.8987		(70.103, 68.93)
x ³ Σ _g ⁻ { ³² S ₂ ³⁴ S ₂ }	0	0	725.668	2.844	0.29541	1.58	21.48	1.889	(g)	(n.p. 115)
	0	0	704.026	2.677	0.27813	1.45	19.59	1.889	(h)	(n.p. 115)

(a) $^3\Pi_2 - ^3\Pi_1 \approx 462 \text{ cm}^{-1}$; (b) $\lambda_o = -11.61 \text{ cm}^{-1}$, $\gamma_o = 0.033 \text{ cm}^{-1}$; (c) $\Delta G_{1/2}$; (d) $\gamma_e \omega_e = -0.005 \text{ cm}^{-1}$;

(e) $^3\Pi_1 - ^3\Pi_2 \approx 130 \text{ cm}^{-1}$; (f) $^3\Delta_2 - ^3\Delta_1 \approx 303.5 \text{ cm}^{-1}$; (g) $\lambda_e = 11.82 \text{ cm}^{-1}$, $\gamma_e = -0.0066 \text{ cm}^{-1}$; (h) $\lambda_e = 11.73 \text{ cm}^{-1}$,

$$\gamma_e = -0.0062 \text{ cm}^{-1}$$

Dissociation energy = $4.4 \pm 0.1 \text{ eV}$, 101.5 kcal/mole , 35300 cm^{-1} (71.107).

Perturbations and General Information

Perturbations by a $B''^3\Pi_u$ state are observed for all vibrational levels. There are three perturbations within each branch.

In emission, the predissociation of the $v'' = 0$ series stops with the (9,0) band at 2828\AA (31.21).

Higher rotational levels of $v' = 17$ of the B - X system and all rotational levels of $v' \geq 18$ are extremely diffuse.

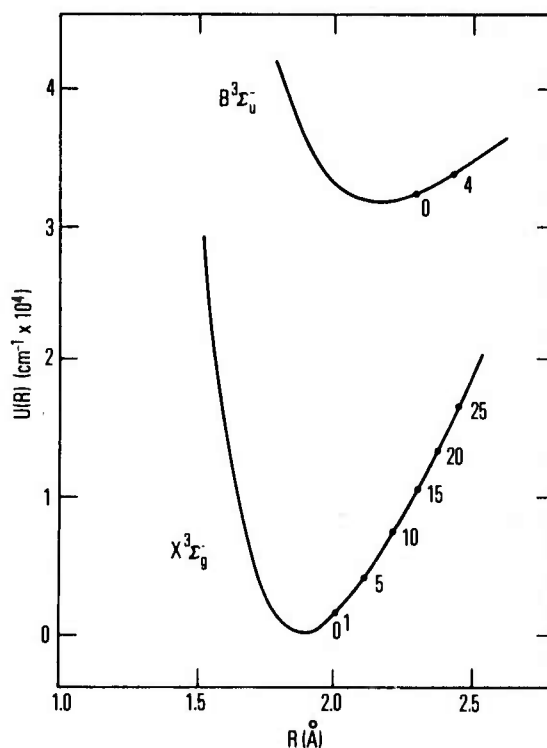
The $B'^3\Pi_g$ and $e^1\Pi_g$ states are predissociated at $v' = 0$ ($B'^3\Pi_2$ for $J \geq 34$ and $B'^3\Pi_2$ for $J \geq 16$) (65.80).

$f^1\Delta_u - a^1\Delta_g$ systems predissociates for $v' \geq 10$ (65.80).

Radiative lifetimes (73.111):

	v'	$\tau(\text{nsec})$
$B^3\Sigma_u^- \rightarrow X^3\Sigma_g^-$	3	20.7
	4	18.3

Potential energy curves - RKR potential (73.112)



BIBLIOGRAPHY

- (27. 1) Fluorescence, Absorption,
B. Rosen,
Z. Physik 43, 69-130
- (29. 2) Resonance Spectra,
P. Swings,
Bull. Intern. Acad. Polon. Sci. A 10, 616-20
- (29. 3) Resonance Series,
P. Swings,
C. R. Acad. Sci. 189, 982-3
- (29. 4) A. M. Taylor,
Trans. Faraday Soc. 25, 929-30
- (30. 5) Resonance Series,
J. Genard,
Bull. Cl. Sci. Acad. Roy. Belg. 16, 923-30
- (30. 6) Resonance Series,
J. Genard,
Bull. Cl. Sci. Acad. Roy. Belg. 16, 1369-77
- (30. 7) Intensity of Resonance Doublet,
P. Swings,
C. R. Acad. Sci. 190, 965-7
- (30. 8) Resonance Doublet,
P. Swings,
C. R. Acad. Sci. 190, 1010-1
- (30. 9) Resonance Spectra,
P. Swings,
C. R. Soc. Polon. Phys. 5, 29-51
- (30. 10) Emission, Predissociation,
H. H. Van Iddekinge,
Nature 125, 858
- (30. 11) Flame Spectra,
V. Kondratjew,
Z. Physik 63, 322-33

- (30. 12) Resonance Spectra,
P. Swings,
Z. Physik 61, 681-99
- (31. 13) Resonance Series,
J. Genard,
Bull. Cl. Sci. Acad. Roy. Belg. 17, 184-90
- (31. 14) Resonance Series,
J. Genard,
Bull. Cl. Sci. Acad. Roy. Belg. 17, 387-99
- (31. 15) Resonance Series,
J. Genard,
Bull. Cl. Sci. Acad. Roy. Belg. 17, 583-92
- (31. 16) Resonance Series,
P. Swings,
Bull. Cl. Sci. Acad. Roy. Belg. 17, 420-4
- (31. 17) Resonance Doublet Intensity,
P. Swings,
Bull. Cl. Sci. Acad. Roy. Belg. 17, 956-71
- (31. 18) Resonance Series,
P. Swings,
Bull. Cl. Sci. Acad. Roy. Belg. 17, 972-4
- (31. 19) Fine Structure of the Resonance Multiplets,
P. Swings and A. Legros,
Bull. Cl. Sci. Acad. Roy. Belg. 17, 808-11
- (31. 20) Resonance Spectra,
J. Fridrichson,
C. R. Acad. Sci. 192, 737-9
- (31. 21) Absorption,
A. Christy and S. M. Naude,
Phys. Rev. 37, 903-19
- (31. 22) Flame Spectra,
A. Fowler and W. M. Vaidya,
Proc. Roy. Soc. A 132, 310-30
- (31. 23) W. C. Curtis and S. Tolansky,
Proc. Univ. Durham Phil. Soc. 8, 323-31

- (31. 24) Resonance Spectra,
J. Fridrickson,
Z. Physik 70, 463-7
- (31. 25) Predissociation,
V. Henri,
Leipziger Vorträge 130
- (34. 26) K. Wieland, M. Wehn, and E. Miescher,
Helv. Phys. Acta 7, 843-9
- (35. 27) Ultraviolet Bands,
B. Rosen and M. Desirant,
Bull. Cl. Sci. Acad. Roy. Belg. 21, 723-35
- (35. 28) Absorption, Predissociation,
I. I. Agarbiceanu,
C. R. Acad. Sci. 200, 385-6
- (35. 29) B - X System, Predissociation,
B. Rosen, M. Desirant, and J. Duchesne,
Phys. Rev. 48, 916
- (36. 30) Infrared Bands,
B. Rosen and F. Bouffioux,
Bull. Cl. Sci. Acad. Roy. Belg. 22, 885-93
- (36. 31) Dissociation Energy,
P. Goldfinger, W. Jeunehomme, and B. Rosen,
Nature 138, 205-6
- (36. 32) Induced Predissociation,
V. Kondratjew and E. Olsson,
Z. Physik 99, 671-6
- (36. 33) B - X System, Rotational Analysis, Dissociation Energy,
E. Olsson,
Z. Physik 100, 656-64
- (37. 34) B - X System, Rotational Analysis,
E. Olsson,
Arkiv Mat. Astron. Fysik B 25, 1-5
- (37. 35) Predissociation,
E. Olsson,
Naturwissenschaften 25, 781-2

- (38.36) B - X System,
E. Olsson,
Arkiv Mat. Astron. Fysik B 26, No. 9
- (38.37) Absorption (4370-3600Å) at High Temperature,
B. Rosen and L. Neven,
J. Chim. Phys. 35, 58-68
- (38.38) Predissociation,
M. Desirant and B. Rosen,
Physica 5, 870-4
- (38.39) Flame Spectra,
E. Schröer,
Z. Phys. Chem. 40, 450-4
- (38.40) Predissociation,
W. Lochte-Holtgreven,
Z. Physik 109, 147-9
- (38.41) Predissociation,
E. Olsson,
Z. Physik 108, 40-4
- (39.42) Absorption,
N. Morguleff,
C. R. Acad. Sci. 208, 273-5
- (40.43) Fluorescence, Energy Transfer,
E. Durand,
J. Chem. Phys. 8, 46-50
- (40.44) Absorption, Induced Predissociation,
G. Herzberg and L. G. Mundie,
J. Chem. Phys. 8, 263-73
- (40.45) Pressure Effect on Predissociation,
B. I. Stepanow,
J. Phys. (USSR) 3, 463-6
- (40.46) Flame Spectra,
D. S. Pavlov,
J. Phys. Chem. (USSR) 14, 601-4
- (40.47) Transfer From OH*,
M. Miyanisi,
Sci. Papers Inst. Phys. Chem. Res. 37, 79-84

- (42. 48) Potential Energy Curves,
J. W. Linnett,
Trans. Faraday Soc. 38, 1-9
- (42. 49) H. Zeise,
Z. Phys. Chem. B 51, 120-5
- (42. 50) S. M. Naude,
Nature 155, 426-7
- (45. 51) Predissociation,
B. Rosen,
Phys. Rev. 68, 124-6
- (45. 52) B - X System, Rotational Analysis,
S. M. Naude,
So. African J. Sci. 41, 128-51
- (47. 53) Flame Spectra,
A. G. Gaydon and G. Whittingham,
Proc. Roy. Soc. A 189, 313-25
- (48. 54) B - X System, Rotational Analysis,
S. M. Naude,
Ann. Phys. 3, 201-22
- (48. 55) Vacuum Ultraviolet Absorption,
R. Maeder,
Helv. Phys. Acta 21, 411-28
- (48. 56) Vacuum Ultraviolet Absorption,
R. Maeder and E. Miescher,
Nature 161, 393
- (49. 57) Paramagnetism,
A. B. Scott,
J. Am. Chem. Soc. 71, 3145-7
- (49. 58) Fluorescence,
P. Pringham,
Fluorescence and Phosphorescence
Interscience Publishers, New York
- (50. 59) B - X System, Perturbations,
S. M. Naude and H. Verleger,
Z. Physik 128, 173-9

- (52. 60) Dissociation Energy,
H. L. Friedman,
J. Chem. Phys. 20, 1046
- (53. 61) B - X System, Rotational Analysis,
K. Ikenoue,
J. Phys. Soc. 8, 646-52
- (56. 62) Ionization Potential,
P. Bradt, F. L. Mohler, and V. H. Dibeler,
J. Res. Nat. Bur. Stand. 57, 223-5
- (59. 63) Dissociation Energy,
L. Brewer,
J. Chem. Phys. 31, 1143-4
- (59. 64) Dissociation Energy,
W. A. Chupka, J. Berkowitz, and C. F. Giese,
J. Chem. Phys. 30, 827-34
- (59. 65) Dissociation Energy,
D. G. H. Marsden,
J. Chem. Phys. 31, 1144-5
- (60. 66) Dissociation Energy,
P. Colin, P. Goldfinger, and M. Jeunehomme,
Nature 187, 408-9
- (60. 67) B - X System, Rotational Analysis,
K. Ikenoue,
Sci. Light 9, 79-97
- (62. 68) Ionization Potential,
P. Hagemann,
C. R. Acad. Sci. 255, 1102-3
- (62. 69) B' → A, B' - A', B - X, e - c Systems, Rotational Analysis,
J. E. Meakin and R. F. Barrow,
Can. J. Phys. 40, 377-9
- (62. 70) Dissociation Energy,
R. Colin and J. Drowart,
J. Chem. Phys. 37, 1120-5
- (62. 71) g - a; h, i → b; C' - X Systems, Vibrational Analysis,
Y. Tanaka and M. Ogawa,
J. Chem. Phys. 36, 726-30

- (62. 72) Dissociation Energy,
T. M. Sugden and A. Demerdache,
Nature 195, 596
- (63. 73) B - X System, Triplet Separation,
R. F. Barrow and J. M. Ketteringham,
Can. J. Phys. 41, 419-23
- (63. 74) Dissociation Energy,
L. Herman and P. Felenbock,
J. Quant. Spectrosc. Radiative Trans. 3, 247-54
- (63. 75) f - a System, vibrational Analysis,
P. B. V. Haranath,
Z. Physik 173, 428-31
- (64. 76) B' - A, B' - A', f - a Systems, Rotational Analysis,
N. A. Narasimham,
Current Sci. 33, 261-3
- (64. 77) f - a System, Rotational Analysis,
N. A. Narasimham and J. K. Brody,
Proc. Indian Acad. Sci. A 59, 345-54
- (64. 78) f - a System, Rotational Analysis,
J. M. Ketteringham and R. F. Barrow,
Proc. Phys. Soc. 83, 330-1
- (64. 79) Dissociation Energy,
P. Colin, P. Goldfinger, and M. Jeunehomme,
Trans. Faraday Soc. 60, 306-16
- (65. 80) f - a System, Rotational Analysis, Isotope Study,
N. A. Narasimham and K. S. Gopal,
Current Sci. 34, 454
- (65. 81) Matrix Isolation,
L. Brewer, G. D. Brabson, and B. Meyer,
J. Chem. Phys. 42, 1385-9
- (65. 82) f - a System, Rotational Analysis, Isotope Study,
N. A. Narasimham and K. M. N. Bhagvat,
Proc. Indian Acad. Sci. 61, 75-9
- (65. 83) Review of Electronic States,
R. F. Barrow and R. P. DuParq,
Elemental Sulfur, B. Meyer, Ed.
Interscience Publ., New York, 251-63

- (66. 84) Dissociation Energy,
J. Drowart and P. Goldfinger,
Quant. Rev. 20, 545-57
- (66. 85) L. Brewer and G. D. Brabson,
"Ultraviolet Fluorescent and Absorption Spectra of S₂ Isolated in
Inert-Gas Matrices,"
J. Chem. Phys. 44, 3274-8
- (66. 86) N. A. Narasimham and K. V. S. R. Apparao,
"Isotope Shifts in the Near Infra-Red Bands of Diatomic Sulphur,"
Nature 210, 1034-5
- (67. 87) N. Basco and A. E. Pearson,
"Reactions of Sulphur Atoms in Presence of Carbon Disulphide,
Carbonyl Sulphide and Nitric Oxide,"
Trans. Faraday Soc. 63, 2684-94
- (67. 88) Matrix Isolation,
B. Petropoulos, O. Dessaux, D. Chaffiol, and P. Goudmand,
C. R. Acad. Sci. 265, 355-8
- (67. 89) System XIII,
G. Lakshminarayana and N. A. Narasimham,
Current Sci. 36, 533
- (68. 90) R. J. Donovan, D. Husain, and P. T. Jackson,
"Transient Species in the Photolysis of Sulphur Monochloride,
including S₂(a¹Δ_g),"
Trans. Faraday Soc. 64, 1798-805
- (68. 91) Ionization Potential,
J. Berkowitz and C. Lifshitz,
J. Chem. Phys. 48, 4346-50
- (68. 92) Dissociation Energy,
P. Budininkas, R. K. Edwards, and P. G. Wahlbeck,
J. Chem. Phys. 48, 2859-66
- (68. 93) f, g - a Systems, Rotational Analysis,
R. F. Barrow and R. P. DuParq,
J. Phys. B 1, 283-8
- (69. 94) D. J. Meschi and A. W. Searcy,
"Investigation of the Magnetic Moments of S₂, Se₂, Te₂, Se₆, and
Se₅ by the Stern-Gerlach Magnetic Deflection Method,"
J. Chem. Phys. 51, 5134-8

- (69.95) W.H. Smith,
"Absolute Transition Probabilities for Some Electronic States of
CS, SO and S₂,"
J. Quant. Spectrosc. Radiative Trans. 9, 1191-9
- (69.96) M. Elbanowski,
"Flash Photolysis of Sulphur Vapour,"
Roc. Chemi. Ann. Soc. Chim. Polon. 43, 1883-91
- (69.97) B - X Systems, Dissociation Energy, Predissociation, Isotope Study,
M. Ogawa and K. R. Yamawakj,
Can. J. Phys. 47, 1805-11
- (69.98) Ionization Potential,
J. Berkowitz and W. A. Chupka,
J. Chem. Phys. 50, 4245-50
- (69.99) C - X System, Rotational Analysis,
R. F. Barrow, R. P. DuParq, and J. M. Ricks,
J. Phys. B 2, 413-8
- (69.100) D - X System,
J. M. Ricks and R. F. Barrow,
J. Phys. B 2, 906-7
- (70.101) Vacuum Ultraviolet Spectra,
R. J. Donovan, D. Husain, and C. D. Stevenson,
Trans. Faraday Soc. 66, 1-9
- (70.102) J. F. Bott and T. A. Jacobs,
"Shock-Tube Study of Radiation From S₂,"
J. Chem. Phys. 52, 3545-50
- (70.103) M. Carleer and R. Colin,
"The $f^1\Delta_u - a^1\Delta_g$ Band System of S₂ in Absorption,"
J. Phys. B 3, 1715-23
- (70.104) A. G. Briggs, R. J. Kemp, L. Batt, and J. H. Holloway,
"Flash Photolysis of Xenon Difluoride, Carbonyl Sulphide and
Nitrogen Trifluoride,"
Spectrochim. Acta 26A, 415-8
- (70.105) A. K. Chaudhry, K. N. Upadhy, and K. P. R. Nair,
"Isotope Shift in the Bands of $B^3\Sigma_u - X^3\Sigma_g$ System of S₂ Molecule,"
Indian J. Pure Appl. Phys. 8, 52-53
- (71.106) A. Tewarson and H. B. Palmer,
"Origins of Chemiluminescent Emission in Low-Pressure Flames
of Sulfur-Containing Compounds,"
Proc. 13th Int. Symp. Combust. 99-107

- (71. 107) B. Rai, J. Singh, and D.K. Rai,
 "Dissociation Energies of S₂, SO, Te₂, SeO and P₂ Molecules,"
Israel J. Chem. 9, 563-8
- (71. 108) S. Durmaz and J.N. Murrell,
 "The Effect of Rotations on the Predissociation Probabilities of
 Diatomic Molecular Spectra,"
Molec. Phys. 21, 209-16
- (72. 109) K.K. Yee, R. F. Barrow, and A. Rogstad,
 "Resonance Fluorescence and Raman Spectra of Gaseous Sulphur,"
J. Chem. Soc. Faraday Trans. 68, 1808-11
- (72. 110) V. S. Zuev, S. B. Kormer, L. D. Mikheev, M. V. Sinitsyn,
 I. I. Sobel'man, and G. I. Startsev,
 "Onset of Inversion in the $1\Sigma_g^+ \rightarrow 3\Sigma_g^-$ Transition of Molecular
 Sulphur Following the Photodissociation of COS,"
JETP Letters 16, 157-8
- (73. 111) K. A. Meyer and D. R. Crosley,
 "Hanle Effect Lifetime Measurements on Selectively Excited
 Diatomic Sulfur,"
J. Chem. Phys. 59, 1933-41
- (73. 112) K. A. Meyer and D. R. Crosley,
 "Franck-Condon Factors From Selectively Excited Resonance
 Fluorescence in the B - X System,"
J. Chem. Phys. 59, 3153-61
- (73. 113) K. A. Meyer and D. R. Crosley,
 "Rotational Satellite Intensities and Triplet Splitting in the B³ Σ_u^-
 State of S₂,"
Can. J. Phys. 51, 2119-24
- (74. 114) F. D. Wayne, P. B. Davies, and B. A. Thrush,
 "The Gas-Phase E. P. R. Spectrum of Diatomic Sulphur Molecules,"
Molec. Phys. 28, 989-96
- (n.p. 115) B - X System, Rotational Analysis, Isotope Study,
 R. F. Barrow and J. M. Ricks,
 Unpublished
- (n.p. 116) X State, Vibrational Constants,
 G. Herzberg,
 Unpublished
- (75. L117) V. S. Zuev, L. D. Mikheev, and V. I. Yalovoi
 "A Photochemical Laser on the S₂($1\Sigma_g^+ - 3\Sigma_g^-$) Electronic Transition,"
Soviet J. Quant. Electronics, 2, 799-806

Sb₂Sb₂Methods of Production and Experimental Technique

Absorption at elevated temperatures (800-1600° C).

Thermal emission and microwave discharge.

Fluorescence excited by Hg.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$A \approx X^1\Sigma_g^+$	Absorption	7500-6000	R			(49.6)
	II	$B \approx X^1\Sigma_g^+$	Absorption	6000-4500	R			(72.9, 49.6)
	III	$D \approx X^1\Sigma_g^+$	Absorption	3400-2830	R	3049.2(6, 2)		(67.8, 35.4)
	IV	$F \approx X^1\Sigma_g^+$	Absorption	2340-2150	R	2222.8(2, 1)		(35.4)
	V	?	Microwaves	8400-7200	V	8315.5, 7788.1		(67.8)
	VI	?	Microwaves	4200-3600	R			(67.8)
	VII	?	Microwaves	3000-2900	R		Triplet structure	(67.8)
	VIII	?	Absorption	< 2170	R	2138.6		(35.4)

Molecule Sb₂

II. B \leftarrow X¹ Σ_g^+ System

Band heads of ¹²¹Sb₂, λ (72.9):

(v', v'')	(5, 0)	(4, 0)	(4, 1)	(3, 0)	(3, 1)
λ	5644.6	5562.0	5496.1	5481.4	5417.5

III. D \leftarrow X¹ Σ_g^+ System

Most intense bands, λ (Intensity):

(v', v'')	(3, 3)	(4, 3)	(7, 4)	(5, 2)	(8, 4)	(6, 2)
λ	3134.7	3114.5	3079.0	3068.9	3059.2	3049.2
(Intensity)	4	4	4	4	4	6

IV. F \leftarrow X¹ Σ_g^+ System

Most intense band heads, λ (Intensity) (35.4):

(v', v'')	(0, 2)	(2, 3)	(0, 1)	(1, 1)	(2, 1)	(2, 0)
λ	2258.5	2249.7	2244.9	2233.4	2222.8	2209.4
(Intensity)	4	2	5	3	7	5

VIII. Band Groups at 2170A

Most intense bands, λ (Intensity) (35.4):

λ	2138.6	2126.8	2115.0	2104.3
(Intensity)	3	2	2	2

SPECTROSCOPIC CONSTANTS

State	T _e	ω _e	x _e ω _e	B _e	α _e × 10 ³	D _e × 10 ⁹	r _e	Remarks	Bibliography
F	44780	226.0	1.17						(35.4)
D	31605	212	0.2						(35.4)
B	19068.9	218.08	0.537	(a) 0.044481		9.1 ^(b)			(72.9, 37.5)
A	14991.5	217.0	0.45						(37.5)
X ¹ Σ _g ⁺	0	269.98	0.588	(a) 0.050039		9.4 ^(b)			(72.9, 37.5)
(a) B ₂ , (b) D ₂									
Dissociation energy = 2.37 ± 0.10 eV, 54.7 kcal/mole, 19120 cm ⁻¹ (73.10).									

Perturbations and General Information

D state is vibrationally perturbed (35.4).

D - X system displays predissociation with a peak at 2842Å. Shorter wavelengths are very diffuse.

BIBLIOGRAPHY

- (33. 1) Fluorescence,
R. Siksna,
C. R. Acad. Sci. 196, 1986-7
- (33. 2) Fluorescence,
J. Genard,
Phys. Rev. 44, 468-9
- (34. 3) S. M. Naude,
Phys. Rev. 45, 280
- (35. 4) Ultraviolet Absorption,
G. Nakamura and T. Shidei,
Jap. J. Phys. 10, 11-25
- (37. 5) Molecular Constants,
G. M. Almy and H. A. Schutz,
Phys. Rev. 51, 62
- (49. 6) L. Gerö and C. Fonö,
J. Chem. Phys. 17, 345-6
- (59. 7) Dissociation Energy,
Yu. Ya. Kuzyakov and V. M. Tatevskii,
Opt. Spectrosc. 7, 467-71
- (67. 8) Microwave Discharge Spectra,
S. Mrozowski and C. Santaram,
J. Opt. Soc. Am. 57, 522-30
- (72. 9) J. Sfeila, P. Perdigon, F. Martin, and B. Femelat,
"The B → X System of Diatomic Antimony,"
J. Molec. Spectrosc. 42, 239-50
- (73. 10) J. Kordis and K. A. Gingerich,
"Mass Spectroscopic Investigation of the Equilibrium Dissociation of
Gaseous Sb₂, Sb₃, Sb₄, SbP, SbP₃, and P₂,"
J. Chem. Phys. 58, 5141-9

Sc₂Spectroscopic Constants

Dissociation energy = 1.12 ± 0.2 eV, 25.9 kcal/mole, 9275 cm^{-1} .

BIBLIOGRAPHY

- (69. 1) K. A. Gingerich,
"Gaseous Metal Borides. I. On the Dissociation Energy of the
Molecules ThB, ThP, and Th₂, and Predicted Dissociation Energies
of Selected Diatomic Transition-Metal Borides,"
High Temp. Sci. 1, 258-67

Methods of Production and Experimental Technique

Absorption at elevated temperatures.

Emission from a microwave discharge in Se vapor.

Laser-induced fluorescence.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	I	$B^3\Sigma_u^- \leftarrow X^3\Sigma_g^-$ $\begin{pmatrix} 0_u^+ - 0_g^+ \\ 1_u - 1_g \end{pmatrix}$	Absorption, fluorescence	6700-3250	R			(72.21, 71.19, 66.11)
	II	$C^3\Sigma_u^- \leftarrow X^3\Sigma_g^-$ $\begin{pmatrix} 0_u^+ - 0_g^+ \\ 1_u - 1_g \\ 1_u - 0_g^+ \end{pmatrix}$	Absorption	1960-1868	V			(70.17)
	III	?	Absorption	1856-1843				(72.20)
	IV	$? \leftarrow X^3\Sigma_g^-$ $(1_u - 1_g)$	Absorption	1845-1820				(70.17)
	V	$? \leftarrow X^3\Sigma_g^-$ $(0_u^+ - 0_g^+)$	Absorption	1826-1812				(70.17)

Molecule Se₂

Se₂

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography
	VI	$n \rightarrow a^1\Delta_g$ $(1_u \rightarrow 2_g)$	oures- nce					(72.20)

Molecule Se₂

I. $B^3\Sigma_u^- \leftarrow X^3\Sigma_g^- (0_u^+ - 0_g^+, 1_u - 1_g)$ Systems

Origins of bands with greatest intensity, λ (66.11):

(v', v'')	(12, 0)	(13, 0)	(14, 0)	(15, 0)	(16, 0)	(17, 0)	(18, 0)
$\lambda(^{80}\text{Se}_2)$	3483.4	3457.5	3432.1	3407.3	3383.3	3360.0	3337.3
$\lambda(^{78}\text{Se}_2)$	3479.8	3453.4	3427.8	3402.9	3378.6	3355.1	3332.4

II. $C^3\Sigma_u^- \leftarrow X^3\Sigma_g^-$ Systems

a. $C(0_u^+) \leftarrow X(0_g^+)$

Strong, diffuse bands with no rotational structure, λ (70.17):

(v', v'')	(0, 2)	(0, 1)	(0, 0)	(1, 0)
λ	1902.04	1888.43	1874.80	1860.36

b. $C(1_u) \leftarrow X(1_g)$

Strong bands with sharp rotational structure, λ (70.17):

v', v''	0	1	2	3
0	1896.49	1910.43	1924.50	1938.7
1	1881.29			1922.87
2	1866.45	1879.96	1893.6	
3	1851.97	1865.25		

c. $C(1_u) \leftarrow X(0_g^+)$

Weak bands with sharp structure, λ (70.17):

(v', v'')	(0, 1)	(0, 0)	(1, 0)
λ	1897.18	1883.38	1868.38

Se₂

III. ? System

Overlaps a continuum centered at ~ 1845Å. Weak bands with sharp structure, λ (70.17):

(v', v'')	(0, 1)	(1, 2)	(0, 0)
λ	1856.53	1855.88	1843.35

IV. ? $\leftarrow X^3\Sigma_g^- (1_u \leftarrow 1_g)$ System

Strong bands, λ (70.17):

(v', v'')	(0, 2)	(1, 3)	(0, 1)	(1, 2)	(0, 0)
λ	1846.23	1844.61	1833.26	1831.69	1820.41

V. ? $\leftarrow X^3\Sigma_g^- (0_u^+ \leftarrow 0_g^+)$ System

Band heads, λ (70.17):

(v', v'')	(0, 0)	(1, 1)	(2, 2)	(3, 3)	(1, 0)	(1, 2)
λ	1826.09	1825.47	1824.85	1824.38	1812.81	1812.28

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e \omega_e$	B_e	$\alpha_e \times 10^4$	$D_e \times 10^8$	r_e	Remarks	Bibliography
1_u	55276.81	430							(70.17)
0_u^+	54752.48	403.9	1.3	0.0924 ^(a)	3.3		^(b) 2.133		(70.17)
?	54239.41	404							(70.17)
$C(0_u^+)$	53339 ^(c)								(70.17)
$C(1_u)$	52709.61	428.0	1.22	0.09647 ^(a)	3.33		2.0893		(70.17)
$q(1_u)^{(d)}$	26991	155	2	0.055 ^(e)					(72.20)
$n(1_u)$	~25985.2	183	~0.75						(72.20)
$B(0_u^+)$	25980.36	246.291	1.016	0.07048	3.45	^(f) 4	2.4464		(66.11)
$B(1_u)$	25912.45	246.42	1.225	0.07086	5.53	^(f) 2	2.4398		(66.11)
$m(1_u)$	~24000	> 154 ^(g)	0.99						(72.20)
$a(2_g)$	~4000	319	0.81						(72.20)
$X(1_g)$	366.7	387.156	0.964	0.09016	2.98	2	2.1630		(71.19, 66.11)

Molecule Se_2

SPECTROSCOPIC CONSTANTS

Molecule Se₂

State	T _e	ω _e	x _e ω _e	B _e	α _e × 10 ⁴	D _e × 10 ⁸	r _e	Remarks	Bibliography
X(0 ⁺ _g)	0	385.302	0.96363	0.08992	2.88	2.4	2.1659		(71.19, 66.11)
(a) B ₀ , (b) r ₀ , (c) T ₀ , (d) analyzed through perturbation of the B state, (e) B ₂ , (f) D ₀ , (g) ΔG _{1/2} Dissociation energy = 3.164 ± 0.002 eV, 72.9 kcal/mole, 25518 cm ⁻¹ (72.20).									

Perturbations and General Information

B(0_u^+) state is perturbed for all vibrational levels, $v \leq 15$ by m, n, and q states. Perturbations for levels of low v are weak (72.20, 63.9).

Both B(0_u^+) and B(1_u) states predissociate (63.9).

Ionization potential (I_p) = 8.88 ± 0.03 eV (69.15).

BIBLIOGRAPHY

- (27. 1) Absorption and Fluorescence,
B. Rosen,
Z. Physik **43**, 69-130
- (34. 2) Isotope Study,
E. Olsson,
Z. Physik **90**, 138-44
- (35. 3) B - X System, Vibrational Analysis,
T. E. Nevin,
Philos. Mag. **20**, 347-54
- (36. 4) B. Rosen and F. Monfort,
Bull. Cl. Sci. Acad. Roy. Belg. **22**, 215-8
- (37. 5) B - X System, Vibrational Analysis,
R. K. Asundi and Y. P. Parti,
Proc. Ind. Acad. Sci. A **6**, 207-28
- (39. 6) B - X System, Vibrational Analysis, Perturbations,
B. Rosen,
Physica **6**, 205-18
- (55. 7) B - X System,
V. Leelavathi and P. T. Rao,
Indian J. Phys. **29**, 1-10
- (63. 8) Dissociation Energy,
D. Detry,
Ind. Chim. Belge **28**, 752-3
- (63. 9) Perturbations and Predissociations,
L. Herman and R. Herman,
Nature **199**, 795
- (66. 10) Dissociation Energy,
J. Berkowitz and W. A. Chupka,
J. Chem. Phys. **45**, 4289-302
- (66. 11) General Analysis,
R. F. Barrow, G. G. Chandler, and C. B. Meyer,
Philos. Trans. Roy. Soc. Lond. A **260**, 395-456

- (66. 12) J. Drowart and P. Goldfinger,
"The Dissociation Energies of the Group VIA Diatomic Molecules,"
Quant. Rev. 20, 545-7
- (68. 13) Dissociation Energy,
P. Budininkas, R.K. Edwards, and P.G. Wahlbeck,
J. Chem. Phys. 48, 2867-9
- (68. 14) Dissociation Energy,
R. Colin and J. Drowart,
Trans. Faraday Soc. 64, 2611-21
- (69. 15) J. Berkowitz and W.A. Chupka,
"Photoionization of High-Temperature Vapors. VI. S₂, Se₂ and Te₂,"
J. Chem. Phys. 50, 4245-50
- (69. 16) D.J. Meschi and A.W. Searcy,
"Investigation of the Magnetic Moments of S₂, Se₂, Te₂ and Se₅ by
the Stern-Gerlach Magnetic Deflection Method,"
J. Chem. Phys. 51, 5134-8
- (70. 17) R.F. Barrow, W.G. Burton, and J.H. Callomon,
"Absorption Spectrum of Gaseous ⁸⁰Se₂ in the Region 51500-55000
cm⁻¹,"
Trans. Faraday Soc. 66, 2685-93
- (70. 18) I.R. Beattie, G.A. Ozin, and R.O. Perry,
"The Gas-Phase Raman Spectra of P₄, P₂, As₄ and As₂. The
Resonance Fluorescence Spectrum of ⁸⁰Se₂. Resonance Fluorescence-
Raman Effects in the Gas-Phase Spectra of Sulphur and I₂. The Effect
of Pressure on the Depolarization Ratios for I₂,"
J. Chem. Soc. A 12, 2071-4
- (71. 19) R.F. Barrow, I.R. Beattie, W.G. Burton, and T. Gilson,
"Resonance Fluorescence Spectra of ⁸⁰Se₂,"
Trans. Faraday Soc. 67, 583-8
- (72. 20) K.K. Yee and R.F. Barrow,
"Absorption and Fluorescence Spectra of Gaseous Se₂,"
J. Chem. Soc. Faraday Trans. 68, 1181-8
- (72. 21) O. Atabek and R. Lefebvre,
"Evaluation of the Level Shifts Produced on the Discrete Levels of
the BO_u⁺ State of the Se₂ Molecule by the Interaction With a Repulsive
State,"
Chem. Phys. Letters 17, 167-171

Methods of Production and Experimental TechniqueAbsorption by flash-photolysis in C₆H₅SiH₃ or BrSiH₃.Emission from discharge in SiH₄ and Xe.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, λ	Remarks	Bibliography
	I	$H^3\Sigma_u^- - X^3\Sigma_g^-$	Flash-photolysis	4526-3863	R	3979.6(4,1)		(71.6, 63.3, 55.2)
	II	$L^3\Pi_g - D^3\Pi_u$	Discharge and flash-photolysis	3695-3489	R	3568.7(0,1) 3496.0(1,1)		(71.6, 55.2)
	III	$K^3\Sigma_u^- - X^3\Sigma_g^-$	Flash-photolysis	3275-3067	R	3202.0(1,0)		(71.6, 63.3)
	IV	$D^3\Pi_u - X^3\Sigma_g^-$	Flash-photolysis	2900-2700		2882.84 2795.80		(70.5)
	V	$N^3\Sigma_u^- - X^3\Sigma_g^-$	Flash-photolysis	2166-2097	R	2138.35(0,0)		(70.4, 63.3)
	VI	$O^3\Sigma_u^- - X^3\Sigma_g^-$	Flash discharge	2200-1800		1874.28(0,0) 1892.21(0,1)		(70.4)
	VII	$P^3\Pi_g - D^3\Pi_u$	Flash discharge	1870-1700	R	1879.9(0,0) 1898.4(0,1)		(70.4)

Molecule Si₂

I. $H^3\Sigma_u^- - X^3\Sigma_g^-$ SystemBand heads, λ (63.3, 55.2):

v', v''	0	1	2	3	4	5	6
0					4427.6	4526.0	
1				4283.1	4375.8	4471.9	
2					4326.0		
3	3942.1						
4	3900.8	3979.6	4060.9				4414.4
5	3863.4						

II. $L^3\Pi_g - D^3\Pi_u$ SystemBand heads, λ (71.6, 55.2):

v', v''	0	1	2	3	4
0		3568.7	3634.4	3710.4	3772.3
1		3496.0	3563.1	3632.2	

III. $K^3\Sigma_u^- - X^3\Sigma_g^-$ SystemBand heads, λ (63.3):

(v', v'')	(0, 0)	(1, 0)	(2, 0)	(3, 0)	(4, 0)
λ	3248.9	3202.0	3157.8	3115.8	3076.1

IV. $D^3\Pi_u - X^3\Sigma_g^-$ System

Several lines have been observed in absorption but have not been identified (70.5):

 λ | 2882.8 | 2838.8 | 2795.8 | 2758.8

Si₂

V. N³Σ_u⁻ - X³Σ_g⁻ System

Band heads, λ (70.4):

v', v''	0	1
0	2138.35	2161.78
1	2117.92	
2	2098.53	
3	2079.75	2101.92
4		2083.53

VI. O³Σ_g⁻ - X³Σ_g⁻ System

Band heads, λ (70.4):

v', v''	0	1	2
0	1874.28	1892.21	
1	1860.53		189.32
2	1847.22	1864.63	

VII. P³Π_g - D³Π_u System

Two red shaded bands have been observed overlapping the O - X system. They are tentatively assigned as follows:

1879.0(0,0)
1898.4(0,1)

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e \omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$P^3\Pi_g$	88219								(70.4)
$L^3\Pi_g$	63059.1			0.2370			2.255		(70.4, 55.2)
$O^3\Sigma_u^-$	53341.94	404.2	3.0	0.2225	3		2.327		
$N^3\Sigma_u^-$	46762.21	458.6	4.8	0.2193	2.5		2.344		(70.4, 63.3)
$D^3\Pi_u$	~35000	547.94	2.43	0.2596	1.55		2.155		(70.4, 55.2)
$K^3\Sigma_u^-$	30768.77	462.6	5.95	0.2185	3.16		2.349		(70.4, 63.4)
$H^3\Sigma_u^-$	^(a) 24311.15	275.30	1.99	0.1712			2.6536		(71.6, 70.4) 63.3, 55.2)
$X^3\Sigma_g^-$	0	510.98	2.02	0.2390	1.3		2.246		(70.4, 63.3)

(a) T_0 Dissociation energy = 3.35 ± 0.2 eV, 75 kcal/mole, 26168 cm^{-1} .

Si₂

Perturbations and General Information

The bands of the K - X and H - X systems exhibit the presence of perturbations. In the H - X system, the (4, 0) band is sharp, but the (5, 0) band is diffuse and does not appear in emission. All the bands of the K - X system are diffuse.

All the levels above $v' = 0$, $J' = 51$ of the L state are predissociated.

The position of the (2, 0) band in the N - X system is displaced somewhat to the red, indicating a perturbation (T0.4).

BIBLIOGRAPHY

- (47. 1) Preliminary Note,
A. R. Downie and R. F. Barrow,
Nature 160, 198
- (55. 2) H - X and L - D Systems,
A. E. Douglas,
Can. J. Phys. 33, 801-10
- (63. 3) H - X, K - X, and N - X Systems,
R. D. Verma and P. A. Warsop,
Can. J. Phys. 41, 152-60
- (70. 4) A. Lagerqvist and C. Malmberg,
"New Absorption Systems of the Si₂ Molecule in the Vacuum Ultra-
violet Region,"
Physica Scripta. 2, 45-9
- (70. 5) D. E. Milligan and M. E. Jacox,
"Infrared and Ultraviolet Spectra of the Products of the Vacuum-
Ultraviolet Photolysis of Silane Isolated in an Argon Matrix,"
J. Chem. Phys. 52, 2594-2608
- (71. 6) I. Dubois and H. Leclercq,
"Absorption Spectrum of Si₂ in the Visible and Near-Ultraviolet
Region,"
Can. J. Phys. 49, 3053-4

Sm₂

Sm₂

Spectroscopic Constants

Dissociation energy = 0.52 ± 0.22 eV, 12 kcal/mole, 4200 cm^{-1} (72.1).

BIBLIOGRAPHY

- (72. 1) A. Kant and S. Lin,
"Dissociation Energies of the Homonuclear Diatomic Rare Earth
Molecules,"
Monatshefte für Chemie 103, 757-63

Sn₂

Sn₂

Band Systems

Bands in the region 4780-4350 Å have been attributed to Sn₂ but may possibly arise from SnCl₂ (62.2).

Spectroscopic Constants

Dissociation energy = 1.99 ± 0.18 eV, 45.8 kcal/mole, 16000 cm^{-1} (62.1).

BIBLIOGRAPHY

- (62. 1) Dissociation Energy by Mass Spectra,
M. Ackerman, J. Drowart, F.E. Stafford, and G. Verhaegen,
J. Chem. Phys. 36, 1557-60
- (62. 2) G. Pannetier and P. Deschamps,
J. Chim. Phys. 59, 517-20

Tb₂

Tb₂

Spectroscopic Constants

Dissociation energy = 1.34 ± 0.35 eV, 31 kcal/mole, 11000 cm^{-1} (72.1).

Tb₂

BIBLIOGRAPHY

- (72. 1) A. Kant and S. Lin,
"Dissociation Energies of the Homonuclear Diatomic Rare Earth
Molecules,"
Monatshefte für Chemie 103, 757-63

Methods of Production and Experimental Technique

Absorption.

Emission from microwave discharge.

Fluorescence, laser-induced fluorescence.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	I	$A 0_u^+ \rightarrow X 0_g^+$	Absorption	5190-4250	R			(69.45, 69.43)
	II	$B 0_u^+ \rightarrow X 0_g^+$	Absorption from discharge	6320-3836	R			(69.43, 69.41, 66.36, 42.31, 38.28, 35.16, 27.1)
	III	$B 0_u^+ \rightarrow X 1_g$	Laser fluo- rescence	5300-6050	R			(72.49)

Molecule Te₂

Te₂

I. A 0_u⁺ ← X 0_g⁺ System (¹³⁰Te₂)

Band origins, λ (69.43):

v', v''	0	1	2	3	4
0					
...					
6					5190.0
7				5089.7	5153.4
8				5054.8	5117.7
9				5020.7	5082.6
10		4868.5		4987.2	5048.4
11		4837.4			5015.0
12		4806.9	4864.2		
13		4777.1	4833.7		
14			4803.8		
15	4665.2		4774.9		
16	4637.9				
17	4611.3		4664.2		
18	4585.1		4637.5		
19	4559.6		4611.4		
20			4585.8		

II. B 0_u⁺ ← X 0_g⁺ System (¹³⁰Te₂)

Band origins, λ (69.45, 69.41):

v', v''	0	1	2	3
0				
...				
5			4449.1	
6			4418.5	4466.6
7		4341.8	4388.5	4436.0
8		4313.2	4359.3	4406.2
9	4240.5	4285.2	4330.7	
10	4213.7	4257.8	4302.7	
11	4187.5	4231.1		
12	4162.0	4205.0		
13	4137.0	4179.6		
14	4112.6			
15	4088.8			
16	4065.7			
17	4043.1			
18	4021.2			
19	3999.8			
20	3979.1			

B 0_u⁺ - X 0_g⁺ System ¹²⁸Te₂

Band origins, λ (69.45, 69.41):

v', v''	0	1	2	...	30	31	32	33
0								
...								
5					6248.7			
6					6188.6	6271.3		
7			4388.8			6210.7	6294.3	
8		4312.9	4359.4				6233.8	6317.7
9		4284.7	4330.2					
10		4257.1						
11	4186.4	4230.3						
12	4160.7	4204.0						
13	4135.6	4178.6						
14	4110.9							
15	4087.2							
16	4064.0							
17	4041.3							
18	4019.2							
19	3997.8							
20	3977.0							

III. B 0_u⁺ - X 1_g System

Band heads, λ (72.58):

	¹²⁸ Te ₂	¹³⁰ Te ₂
v'', v'	0	0
0		
...		
5	5350.0	
6	5421.1	
7	5493.6	5492.7
8	5567.9	5566.1
9	5643.8	5641.6
10	5721.6	5718.8
11	5800.9	5797.8
12	5882.3	5878.7
13	5965.6	5961.1
14	6050.8	6045.5
15	6138.2	
16	6227.7	

SPECTROSCOPIC CONSTANTS

Molecule Te_2

State	T_e	ω_e	$x_e \omega_e$	$B_e \times 10^2$	$\alpha_e \times 10^4$	$D_e \times 10^9$	r_e	Remarks	Bibliography
$^{130}\text{Te}_2$									
$B 0_u^+$	22207.4	162.3	0.45	3.254	1.25		2.8244	$y_e \omega_e = -11.09 \times 10^{-3}$	(72.48, 69.45, 69.43)
$A 0_u^+$	19450.8	143.6	0.45	3.124	1.30		2.8824	$y_e \omega_e = -3.892 \times 10^{-3}$	(72.48, 69.43)
$X 1_g$	2234	250.00	0.547	3.968(a)	1.06(a)				(72.49, 69.43)
$X 0_g^+$	0	247.07	0.515	3.968	1.06	4.4	2.5774	$y_e \omega_e = -0.55 \times 10^{-3}$	(72.48, 69.43)
$^{128}\text{Te}_2$									
$B 0_u^+$	22285.6 ^(b)			3.3121	1.41		2.82442		(72.48, 69.45, 69.43)
$A 0_u^+$	19450			3.1740	1.32		2.88226		(72.48, 69.45, 69.43)
$X 1_g$	2228.5	251.26	0.536	4.0299(a)	1.03(a)				(72.48, 69.45, 69.43)
$X 0_g^+$	0			4.0299	1.03	4.1	2.55766		(72.48, 69.45, 69.43)

Molecule Te_2 [illegible]

Te₂

Perturbations and General Information

RKR potential energy curve (n.p. 50) for ¹²⁸Te₂ X 0_g⁺ state:

T _e = 0 cm ⁻¹	v	T _e + E(v) cm ⁻¹	r _{min} (Å)	r _{max} (Å)
	0	124.35	2.51335	2.60548
	1	372.26	2.48249	2.64234
	2	619.12	2.46205	2.66878
	3	864.92	2.44591	2.69096
	4	1109.65	2.43229	2.71065
	5	1353.33	2.42037	2.72867
	6	1595.94	2.40971	2.74547
	7	1837.49	2.40000	2.76133
	8	2077.96	2.39108	2.77646
	9	2317.36	2.38286	2.79084
	10	2555.68	2.37513	2.80484
	11	2792.92	2.36782	2.81846
	12	3029.09	2.36095	2.83165
	13	3264.16	2.35441	2.84456
	14	3498.15	2.34819	2.85715
	15	3731.05	2.34227	2.86953

RKR potential energy curve (n.p. 50) for ¹²⁸Te₂ A 0_u⁺ state:

T _e = 19450 cm ⁻¹	v	T _e + E(v) cm ⁻¹	r _{min} (Å)	r _{max} (Å)
	0	72.24	2.82474	2.94564
	1	216.01	2.78550	2.99546
	2	358.83	2.75988	3.03171
	3	500.67	2.73987	3.06242
	4	641.50	2.72311	3.08994
	5	781.30	2.70854	3.11533
	6	920.05	2.69557	3.13918
	7	1057.72	2.68383	3.16188
	8	1194.28	2.67307	3.18367
	9	1329.73	2.66317	3.20455
	10	1464.02	2.65389	3.22501
	11	1597.14	2.64511	3.24506
	12	1729.07	2.63686	3.26464
	13	1859.78	2.62900	3.28393
	14	1989.24	2.62153	3.30290
	15	2117.43	2.61435	3.32167

FKR potential energy curve (n.p. 50) for $^{128}\text{Te}_2$ B 0_u^+ state:

$T_e = 22285.5 \text{ cm}^{-1}$	v	$T_e + E(v) \text{ cm}^{-1}$	$r_{\min}(\text{\AA})$	$r_{\max}(\text{\AA})$
	0	81.68	2.77021	2.88390
	1	244.31	2.73361	2.93102
	2	405.92	2.70967	2.96521
	3	566.44	2.69099	2.99420
	4	725.80	2.67543	3.02028
	5	883.93	2.66201	3.04448
	6	1040.77	2.65009	3.06729
	7	1196.24	2.63915	3.08889
	8	1350.28	2.62870	3.10929
	9	1502.76	2.61904	3.12893
	10	1653.68	2.60899	3.14728
	11	1803.11	2.60141	3.16717
	12	1950.68	2.59302	3.18565
	13	2096.49	2.58499	3.20395
	14	2240.49	2.57882	3.22345
	15	2382.58	2.57212	3.24213

Franck-Condon factors for $^{128}\text{Te}_2$ ($A 0_u^+ - X 0_g^+$) (n.p. 50):

	12	13	14	15	16	17	18	19
0	4.985-2	6.959-2	8.846-2	1.032-1	1.110-1	1.102-1	1.014-1	8.679-2
1	7.975-2	7.178-3	5.109-2	2.559-2	5.839-3	2.330-4	1.094-2	3.319-2
2	3.035-2	7.032-3	4.068-4	1.415-2	3.767-2	5.356-2	5.064-2	3.155-2
3	4.838-4	1.598-2	3.871-2	4.614-2	3.100-2	8.307-3	2.854-4	1.440-2
4	2.969-2	4.213-2	2.891-2	6.186-3	1.449-3	1.988-2	3.861-2	3.526-2
5	3.601-2	1.414-2	2.368-6	1.316-2	3.354-2	3.128-2	9.981-3	2.531-4
6	7.044-3	1.933-3	2.217-2	3.304-2	1.643-2	2.123-4	1.101-2	3.076-2
7	3.998-3	2.552-2	2.833-2	7.349-3	1.782-3	2.138-2	2.942-2	1.135-2
8	2.536-2	2.501-2	3.738-3	5.140-3	2.536-2	2.256-2	2.672-3	5.871-3
9	2.428-2	3.104-3	6.396-3	2.556-2	1.740-2	2.713-4	1.184-2	2.638-2
10	4.517-3	5.263-3	2.444-2	1.540-2	2.557-6	1.458-2	2.409-2	6.246-3

Franck-Condon factor followed by factor of ten

Te₂

Franck-Condon factors for ¹²⁸Te₂ (B 0_u⁺ - X 0_g⁺) (n.p. 50):

	9	10	11	12	13	14	15	16
0	8.506-2	1.101-1	1.267-1	1.305-1	1.208-1	1.001-1	7.702-2	5.374-2
1	8.231-2	5.196-2	1.833-2	5.264-4	8.427-3	3.676-2	7.006-2	9.305-2
2	7.989-3	1.866-3	2.622-2	5.616-2	6.270-2	4.059-2	1.115-2	1.710-4
3	1.719-2	4.769-2	5.101-2	2.326-2	6.824-4	1.165-2	4.208-2	5.623-2
4	4.911-2	3.233-2	3.279-3	7.950-3	3.754-2	4.508-2	1.981-2	1.478-4
5	2.209-2	1.318-5	1.961-2	4.190-2	2.498-2	8.072-4	1.316-2	4.003-2
6	1.247-4	2.365-2	3.789-2	1.228-2	1.716-3	2.766-2	3.619-2	1.062-2
7	2.161-2	3.507-2	8.070-3	5.026-3	3.186-2	2.546-2	1.000-3	1.360-2
8	3.429-2	8.942-3	5.096-3	3.117-2	1.933-2	4.950-5	2.135-2	3.063-2
9	1.396-2	2.415-3	2.848-2	1.842-2	2.691-4	2.322-2	2.494-2	1.082-3
10	3.614-5	2.312-2	2.132-2	3.220-6	2.129-2	2.269-2	2.589-4	1.739-2

Franck-Condon factor followed by factor of ten

Perturbations of the v = 0 level of the B 0_u⁺ state have been observed.

Ionization cross sections = $17.46 \pm 0.48 \times 10^{-6} \text{ cm}^2$ (66.37).

BIBLIOGRAPHY

- (27. 1) B \neq X System in Absorption and Fluorescence,
E. Rosen,
Z. Physik 43, 69-130
- (29. 2) Resonance Series,
W. Kessel,
C. R. Acad. Sci. 189, 94-6
- (29. 3) Resonance Series,
W. Kessel,
C. R. Soc. Polon. Phys. 4, 175-82
- (29. 4) Resonance Series,
W. Kessel,
C. R. Soc. Polon. Phys. 4, 183-91
- (31. 5) Fluorescence,
J. Genard,
Bull. Cl. Sci. Acad. Roy. Belg. 17, 1241-8
- (31. 6) Resonance Series,
A. Legros,
Bull. Cl. Sci. Acad. Roy. Belg. 17, 816-22
- (31. 7) Resonance Series,
J. Pierard,
Bull. Cl. Sci. Acad. Roy. Belg. 17, 974-9
- (31. 8) Resonance Series,
P. Swings and J. Genard,
Bull. Cl. Sci. Acad. Roy. Belg. 17, 1099-106
- (32. 9) Resonance Series,
J. Pierard,
Bull. Cl. Sci. Acad. Roy. Belg. 18, 180-5
- (32. 10) Resonance Series,
J. Pierard and M. Migeotte,
Bull. Cl. Sci. Acad. Roy. Belg. 18, 246-55
- (32. 11) Absorption and Predissociation,
E. Hirschlaff,
Z. Physik 75, 315-24

- (33. 12) Fluorescence Excited by Magnetic Field,
R. Smoluchewski,
Z. Physik 85, 191-200
- (34. 13) Resonance Series,
W. Kessel,
Acta Phys. Polon. 3, 505-12
- (34. 14) Induced Predissociation,
V. Kondratjew and A. Lauris,
Z. Physik 92, 741-6
- (35. 15) Effect of Magnetic Field,
I. I. Agarbiceanu,
C. R. Acad. Sci. 200, 385-6
- (35. 16) B → X System, Vibrational Analysis, Isotope Effect,
E. Olsson,
Z. Physik 95, 215-20
- (36. 17) Fluctuations,
M. Desirant and A. Minne,
Bull. Cl. Sci. Acad. Roy. Belg. 22, 646-58
- (36. 18) Fluctuations,
B. Rosen and F. Bouffioux,
Bull. Cl. Sci. Acad. Roy. Belg. 22, 885-93
- (36. 19) Fluctuations,
M. Desirant and A. Minne,
C. R. Acad. Sci. 202, 1272-3
- (36. 20) Dissociation Energy,
P. Goldfinger, W. Jeunehomme, and B. Rosen,
Nature 138, 205-6
- (36. 21) Te + Te Recombination Continuum,
R. Rompe,
Phys. Z. 37, 807-8
- (36. 22) Te + Te Recombination Continuum,
R. Rompe,
Z. Phys. 101, 214-33
- (37. 23) Resonance Series. Isotope Effect,
B. Rosen and J. Mat,
Bull. Cl. Sci. Acad. Roy. Belg. 23, 626-45

- (37. 24) Induced Predissociation by Magnetic Field,
E. Olsson,
C. R. Acad. Sci. 204, 1182-4
- (37. 25) Electron Diffraction,
L. R. Maxwell and V. M. Mosley,
Phys. Rev. 51, 648
- (38. 26) Fluorescence Polarization,
S. Mrozowski,
Acta Phys. Polon. 7, 45-8
- (38. 27) Ultraviolet System,
C. Shin-Piaw,
Ann. Physique 10, 173-290
- (38. 28) B - X System, Vibrational Analysis, Isotope Effect; Effect of Magnetic Field on Induced Predissociation,
E. Olsson,
Thesis, Stockholm
- (40. 29) Electron Diffraction,
L. R. Maxwell and V. M. Mosley,
Phys. Rev. 57, 21-3
- (40. 30) Te₂ \rightleftharpoons 2Te; Dissociation Energy,
H. Zeise,
Z. Elektrochem. 46, 38-41
- (42. 31) Determination of $x_e \omega_e$,
R. Migeotte,
Bull. Soc. Roy. Sci. Liege 11, 48-53
- (42. 32) Ultraviolet System Between 2450-1950 Å,
R. Migeotte,
Mem. Soc. Roy. Sci. Liege 5, 549-75
- (42. 33) Potential Energy, Internuclear Distance,
Y. Tanaka and T. Takamine,
Sci. Papers Inst. Phys. Chem. Res. Japan, 39, 437-46
- (44. 34) Predissociation in the B State,
R. Migeotte and B. Rosen,
Bull. Soc. Roy. Sci. Liege 13, 248-54
- (45. 35) Induced Predissociation,
B. Rosen,
Phys. Rev. 68, 124-6

Te₂

- (66. 36) R. P. duParcq and R. F. Barrow,
"The Internuclear Distance in the Te₂ Molecule,"
Chem. Com. 9, 270
- (66. 37) R. F. Pottie,
"Cross Sections for Ionization by Electrons. I. Absolute Ionization
Cross Sections of Zn, Cd, and Te₂, II. Comparisons of Theoretical
With Experimental Values for Atoms and Molecules,"
J. Chem. Phys. 44, 916-22
- (66. 38) J. Drowart and P. Goldfinger,
"The Dissociation Energies of the Group VIA Diatomic Molecules,"
Quant. Rev. 20, 545-57
- (67. 39) P. Budininkas,
"Dissociation Energies of Gaseous Diatomic Sulfur, Selenium and
Tellurium,"
Thesis, Illinois Institute of Technology
- (68. 40) P. Budininkas,
"Dissociation Energies of Group VIA Gaseous Homonuclear Diatomic
Molecules. III. Tellurium,"
J. Chem. Phys. 48, 2870-3
- (69. 41) B - X System of ¹³⁰Te₂, Rotational Analysis,
B. L. Jha and D. R. Rao,
Chem. Phys. Letters 3, 175-6
- (69. 42) J. Berkowitz and W. A. Chupka,
"Photoionization of High-Temperature Vapors. VI. S₂, Se₂, and
Te₂,"
J. Chem. Phys. 50, 4245-50
- (69. 43) A, B - X Systems of ¹²⁸Te₂, ¹³⁰Te₂, Rotational Analysis,
R. P. duParcq,
Thesis, Oxford
- (69. 44) D. J. Meschi and A. W. Searcy,
"Investigation of the Magnetic Moments of S₂, Se₂, Te₂ and Se₅ by
the Stern-Gerlach Magnetic Deflection Method,"
J. Chem. Phys. 51, 5134-8
- (69. 45) B. L. Jha, K. V. Subbaram, and D. R. Rao,
"Electronic Spectra of ¹³⁰Te₂ and ¹²⁸Te₂,"
J. Molec. Spectrosc. 32, 383-97

- (71.46) E. O. Degenkolb, H. Mayfarth, and J. I. Steinfeld,
"Laser-Excited Fluorescence of Tellurium Vapor,"
Chem. Phys. Letters 2, 288-90
- (71.47) B. Rai, J. Singh, and D. K. Rai,
"Dissociation Energies of S₂, SO, Te₂, SeO and P₂,"
Israel J. Chem. 9, 563-8
- (72.48) R. F. Barrow and R. P. duParcq,
"Rotational Analysis of the A 0_u⁺, B 0_u⁺ - X 0_g⁺ Systems of Gaseous Te₂,"
Proc. Roy. Soc. London A 327, 279-287
- (72.49) K. K. Yee and R. F. Barrow,
"Observations on the Absorption and Fluorescence Spectra of Gaseous
Te₂,"
J. Chem. Soc. Faraday Trans. II 68, 1397-1403
- (n.p. 50) R. F. Barrow,
Private communication (see 72.49)

Th₂

Th₂

Spectroscopic Constants

Dissociation energy = 2.95 ± 0.35 eV, 68 kcal/mole, 24000 cm^{-1} (69.1).

BIBLIOGRAPHY

- (69. 1) K. A. Gingerich,
"Gaseous Metal Borides. I On the Dissociation Energy of the
Molecules ThB, ThP, and Th₂, and Predicted Dissociation Energies
of Selected Diatomic Transition-Metal Borides,"
High Temp. Sci. 1, 258-267

Ti₂

Ti₂

Spectroscopic Constants

Dissociation energy = 1.15 ± 0.17 eV, 28.3 kcal/mol, 9000 cm⁻¹ (69.2).

BIBLIOGRAPHY

- (64. 1) A. Kant and B. Strauss,
"Dissociation Energies of Diatomic Molecules of the Transition
Elements. II. Titanium, Chromium, Manganese, and Cobalt,"
J. Chem. Phys. 41, 3806-8
- (69. 2) A. Kant and S. Lin,
"Dissociation Energies of Ti₂ and V₂,"
J. Chem. Phys. 51, 1644-7
- (69. 3) K. A. Gingerich,
"Gaseous Metal Borides. I. On the Dissociation Energy of the
Molecules ThB, ThP, and Th₂, and Predicted Dissociation Energies
of Selected Diatomic Transition-Metal Borides,"
High Temp. Sci. 1, 258-67

Tl₂

Tl₂

Methods of Production and Experimental Technique

Absorption.

Emission from a hollow cathode and a King furnace.

Band Systems

Five groups of bands have been observed in emission and absorption (65.5, 65.4, 31.2, 31.1).

I. "Red System" - 6500-4900Å

λ in emission (65.5):

v', v''	0	1	2	3	4
0	6320.3	6375.5	6428.4	6483.0	6537.2
1	6285.4	6339.1	6393.0		
2	6252.0				

The conclusions on the origin of this band system are uncertain. Initial investigation gives $\omega' \sim 88 \text{ cm}^{-1}$ and $\omega'' \approx 136 \text{ cm}^{-1}$ (65.5).

II. 4635-3680Å System

Emission

In emission, the band head appears to be at $\lambda \sim 3770.7\text{Å}$, with band maxima at:

$$\lambda = 4635 | 4405 | 4308 | 4237 | 4187 | 4133 | 4047 | 4004$$

diffuse and weak maxima at:

$$\lambda = 3923 | 3857 | 3800$$

Absorption

Extensive tables of lines seen in absorption (4400-4200Å) are given in (65.5). There are two tentative assignments given to some of them.

Assignment I:

v', v''	0	1	2	3	4	5	6	7	8
0	4269.9	4287.1	4302.2	4322.2	4340.3				
1		4263.7		4299.1	4360.2	4335.4	4354.2	4372.4	4390.3
2			4251.6	4276.8	4293.9				
3				4255.3	4271.9				
4					4250.8				

Tl₂

Assignment II:

v', v''	0	1	2	3	4	5	6	7
0	4400.2	4419.0						
1		4394.3	4412.6	4431.9				
2		4370.2		4406.5	4425.1			
3					4401.9	4420.4		
4						4396.0	4414.2	
5						4372.4	4390.3	4408.7

III. 3776-3260Å System

Bands are symmetrical around the lines at 3529 and 3519Å. Maxima at ~ 3600Å.

IV. 2850-2740Å System

Bands are asymmetrical around the 2768Å line with an apparent head at 2766.3Å.

V. Visible Continua - 2768Å System

This system arises from the broadening of the lines 3230, 3092, 2922-2919Å. Maxima at $\lambda \sim 3446|3156|3050\text{Å}$.

Spectroscopic Constants

Dissociation energy = <0.9 eV, <21 kcal/mole, <7300 cm⁻¹ (57.3).

BIBLIOGRAPHY

- (31. 1) Hollow Cathode,
H. Hamada,
Nature 127, 555
- (31. 2) Hollow Cathode,
H. Hamada,
Philos. Mag. 12, 50-67
- (57. 3) Dissociation Energy by Mass Spectra,
J. Drowart and R. E. Honig,
J. Chem. Phys. 61, 980-5
- (65. 4) Thermal Emission and Absorption Bands,
D. E. S. Ginter, M. L. Ginter, and K. K. Innes,
J. Phys. Chem. 69, 2480-3
- (65. 5) D. E. S. Ginter,
"Electronic Spectra of the Homonuclear Molecules of the Group III
Metals,"
Thesis, Vanderbilt University

Tm_2

Tm_2

Spectroscopic Constants

Dissociation energy = 0.52 ± 0.17 eV, 12 kcal/mole, 4200 cm^{-1} (72.2).

BIBLIOGRAPHY

- (71. 1) S. Lin and A. Kant,
"Dissociation Energies of Diatomic Rare Earth Molecules Dy₂, Ho₂,
Er₂, Tm₂, and Yb₂,"
Army Materials and Mechanics Research Center, TR No. 71-34
- (72. 2) A. Kant and S. Lin,
"Dissociation Energies of Homonuclear Diatomic Molecules of the
Rare Earths,"
Monatshefte für Chemie 103, 757-63

U₂Spectroscopic Constants

Dissociation energy = 1.73 ± 0.43 eV, 40 kcal/mole, 14000 cm^{-1} (69.1).

U₂

BIBLIOGRAPHY

- (69. 1) K. A. Gingerich,
"Gaseous Metal Borides. I. On the Dissociation Energy of the
Molecules ThB, ThP, and Th₂, and Predicted Dissociation Energies
of Selected Diatomic Transition-Metal Borides,"
High Temp. Sci. 1, 258-67

V₂Spectroscopic Constants

Dissociation energy = 2.49 ± 0.13 eV, 57.5 kcal/mole, 20100 cm^{-1} (69.1).

BIBLIOGRAPHY

- (69. 1) A. Kant and S. Lin,
"Dissociation Energies of Ti₂ and V₂,"
J. Chem. Phys. 51, 1644-7

Methods of Production and Experimental Technique

Absorption.

Emission from electron beam discharge, laser pumping, α particles, x rays.

BAND SYSTEMS

	System	Transition	Sources	Wave- length limits	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography
	I	?	Electron beam, X rays	5000-2600			Continuum	(67.7)
	II	$1,3\Sigma_u^+ \leftarrow X^1\Sigma_g^+$ $\begin{pmatrix} 0_u^+ - 0_g^+ \\ 1_u - 0_g^+ \end{pmatrix}$	Electron beam	2250-1470			Continuum	(74.33, 72.14, 65.4, 55.3, 55.2)
	III	$1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$ $(0_u^+ - 0_g^+)$	Electron beam	1305-1295				(74.33, 72.14)
	IV	$1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$ $(0_u^+ - 0_g^+)$	Electron beam	1207-1192				(74.33, 72.14)
	V	$3\Sigma_u^+ \leftarrow X^1\Sigma_g^+$ $(1_u - 0_g^+)$	Electron beam	1192-1191				(74.33, 72.14)

Molecule Xe₂

Xe₂

II. $1,3\Sigma_u^+ \leftarrow X^1\Sigma_g^+ (0_u^+, 1_u - 0_g^+)$ Systems

Upper state correlated to $5p^6 1S_0 + 6s(3/2)_1^0$ (74.33, 72.14).

III. $1\Sigma_u^+ \leftarrow X^1\Sigma_g^+ (0_u^+ - 0_g^+)$ System

Upper state correlated to $5p^6 1S_0 + 6s'(1/2)_1^0$ (74.33, 72.14).

IV. $1\Sigma_u^+ \leftarrow X^1\Sigma_g^+ (0_u^+ - 0_g^+)$ System

Upper state correlated to $5p^6 1S_0 + 5d(3/2)_1^0$ (74.33, 72.14).

Transition	Source	Wavelength Limits	Exposure	Band Head	Remarks	Reference
II	Electron beam	1300-1400				(74.33, 72.14)
		1300-1400				
III	Electron beam	1300-1400				(74.33, 72.14)
		1300-1400				
IV	Electron beam	1300-1400				(74.33, 72.14)
		1300-1400				
V	Electron beam	1300-1400				(74.33, 72.14)
		1300-1400				

SPECTROSCOPIC CONSTANTS

State	T_e	ω_e	$x_e \omega_e$	B_e	$\alpha_e \times 10^3$	$D_e \times 10^6$	r_e	Remarks	Bibliography
$X^1\Sigma_g^+$ (0^+)	0	~ 21.26	~ 0.75	~ 0.013	~ 0.4		~ 4.45	$y_e \omega_e \sim 0.008$	(70.9)
Dissociation energy $\sim 2.4 \times 10^{-2}$ eV, 0.55 kcal/mole, 192.02 cm^{-1} (70.9).									

Molecule Xe_2

Xe_2

Perturbations and General Information

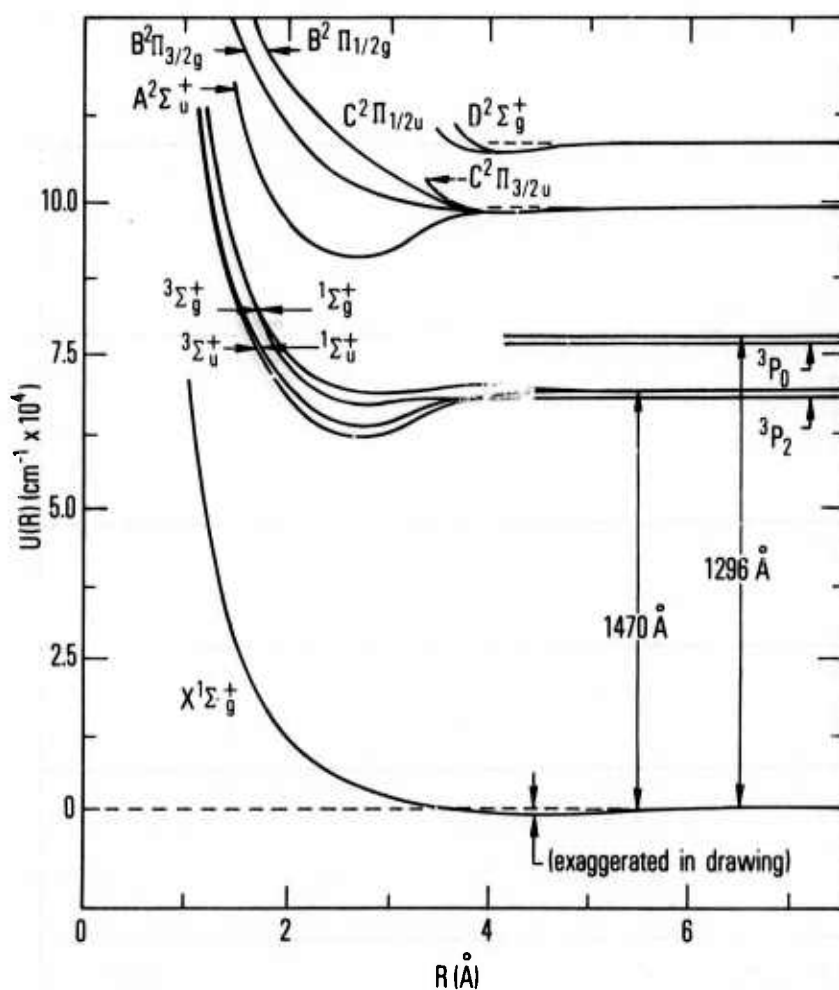
Quenching of $\text{Xe}_2^{1,3}\Sigma_u^+$ by Xe: $\sigma \approx 10^{-17} \text{ cm}^2$ (73.25).

Laser action observed on the $^{1,3}\Sigma_u^+ \rightarrow X^1\Sigma_g^+$ transition at $1720 \pm 10 \text{ \AA}$ (74.36, 74.31, 74.30, 73.28, 73.23, 73.22, 73.21, 73.20, 73.19, 73.18).

Radiative lifetime of $^{1,3}\Sigma_u^+ - X^1\Sigma_g^+$

$$\begin{aligned} \tau &= 23 \text{ nsec (74.32)} \\ &= 130 \text{ nsec (73.18)}. \end{aligned}$$

Potential energy curves - estimated (70.10):



BIBLIOGRAPHY

- (54. 1) Y. Tanaka and M. Zelikoff,
"Continuous Emission Spectrum of Xenon in the Vacuum Ultraviolet
Region,"
J. Opt. Soc. Am. 44, 254-5
- (55. 2) Condensed Discharge,
Y. Tanaka,
J. Opt. Soc. Am. 45, 710-3
- (55. 3) Weak Discharge,
P.G. Wilkinson and Y. Tanaka,
J. Opt. Soc. Am. 45, 344-9
- (65. 4) Microwave Discharge,
P.G. Wilkinson and E.T. Byram,
Applied Optics 4, 581-8
- (67. 5) J.F. Prince and W.W. Robertson,
"Visible Continua in Xenon, Krypton, and Neon,"
J. Chem. Phys. 46, 3309-13
- (67. 6) P.G. Wilkinson,
"The Mechanism of the Argon Emission Continuum in the Vacuum
Ultraviolet. I,"
Can. J. Phys. 45, 1715-27
- (67. 7) B. Brocklehurst,
"Luminescence of Gases Excited by High Energy Radiation. Part 2.
Emission Spectra of Molecular Xenon,"
Trans. Faraday Soc. 63, 274-81
- (68. 8) L.L. Nichols and W. Vali,
"Pressure Dependence of the Xenon Continuum Radiation Decay Rate,"
J. Chem. Phys. 49, 814-7
- (70. 9) J.P. Morucci and A. Lansart,
"Investigation of Light Emission by Electron Avalanches in Binary
Mixtures Where Xenon is the Parent Constituent. Attempted Interpre-
tation of the Visible Continuum Emitted by Xenon,"
IEEE Trans. Nucl. Sci. 17, 95-106
- (70. 10) R.S. Mulliken,
"Potential Curves of Diatomic Rare-Gas Molecules and Their Ions,
With Particular Reference to Xe₂,"
J. Chem. Phys. 52, 5170-80

- (71. 11) I. V. Kozinskaya and L. P. Polozova,
"Molecular Absorption of Xenon in the Vacuum Ultraviolet,"
Optics & Spectroscopy 30, 853-8
- (71. 12) C. G. Freeman, M. J. McEwan, R. F. C. Claridge, and L. F. Phillips,
"Band Fluorescence of Xenon,"
Chem. Phys. Letters 10, 530-2
- (71. 13) Xe₂ Laser,
N. G. Basov, V. A. Danilychev, and Yu. M. Papov,
Sov. J. Quant. Electron. 1, 18-20
- (72. 14) M. C. Castex and N. Damany,
"Absorption Spectrum of the Xenon Molecule in the Vacuum Ultra-
violet Region,"
Chem. Phys. Letters 13, 158-161
- (72. 15) O. Cheshnovsky, B. Raz, and J. Jortner,
"Temperature Dependence of Rare Gas Molecular Emission in the
Vacuum Ultraviolet,"
Chem. Phys. Letters 15, 475-9
- (72. 16) Xe₂ Laser,
H. A. Koehler, L. J. Ferderber, D. L. Redhead, and P. J. Ebert,
Appl. Phys. Letters 21, 198-9
- (73. 17) A. Gedanken, B. Raz, and J. Jortner,
"Emission Spectra of Homonuclear Diatomic Rare Gas Molecules in
Solid Neon,"
J. Chem. Phys. 59, 1630-3
- (73. 18) S. C. Wallace, R. T. Hodgson, and R. W. Dreyfus,
"Excitation of Vacuum Ultraviolet Emission From High-Pressure
Xenon by Relativistic Electron Beams,"
Appl. Phys. Letters 23, 22-24
- (73. 19) S. C. Wallace, R. T. Hodgson, and R. W. Dreyfus,
"Short Pulse Excitation of a Xenon Molecular Dissociation Laser at
172.9 nm by Relativistic Electrons,"
Appl. Phys. Letters 23, 672-4
- (73. 20) E. R. Ault, M. L. Bhaumik, W. M. Hughes, R. J. Jensen, C. P. Robinson,
A. C. Kolb, and J. Shannon,
"Xenon Molecular Laser in the Vacuum Ultraviolet,"
IEEE J. Quant. Electronics 10, 1031-2

- (73.21) J. B. Gerardo and A. W. Johnson,
"1730-Å Radiation Dominated by Stimulated Emission From High-
Pressure Xenon,"
J. Appl. Phys. 44, 4120-4
- (73.22) M. Novaro and F. Lagarde,
"Evidence of Stimulated Emission From Xenon Under Pressure,"
C.R. Acad. Sci. B 277, 671-3
- (73.23) P. W. Hoff, J. C. Swingle, and C. K. Rhodes,
"Demonstration of Temporal Coherence, Spatial Coherence, and
Threshold Effects in the Molecular Xenon Laser,"
Optics Comm. 8, 128-131
- (73.24) F. H. Mies,
"Stimulated Emission and Population Inversion in Diatomic Bound-
Continuum Transitions,"
Molec. Phys. 26, 1233-46
- (73.25) D. J. Bradley, M. H. R. Hutchinson, and H. Koetser,
"Quenching of Vacuum Ultraviolet Fluorescence Emission From
Electron Beam Excited Quasi-Molecular Xenon,"
Optics Comm. 7, 187-190
- (73.26) P. W. Hoff, J. C. Swingle, and C. K. Rhodes,
"Observations of Stimulated Emission From High-Pressure Krypton
and Argon/Xenon Mixtures,"
Appl. Phys. Letters 23, 245-6
- (73.27) K. K. Docken and T. P. Schafer,
"Spectroscopic Information on Ground-State Ar₂, Kr₂, and Xe₂
From Interatomic Potentials,"
J. Molec. Spectrosc. 46, 454-9
- (73.28) S. E. Harris, A. H. Kung, E. A. Stappaerts, and J. F. Young,
"Stimulated Emission in Multiple-Photon-Pumped Xenon and Argon
Excimers,"
Appl. Phys. Letters 23, 232-4
- (73.29) O. Cheshnovsky, B. Raz, and J. Jortner,
"Electronic Energy Transfer in Rare Gas Mixtures,"
J. Chem. Phys. 57, 3301-7
- (74.30) W. M. Hughes, J. Shannon, and R. Hunter,
"Efficient High-Energy-Density Molecular Xenon Laser,"
Appl. Phys. Letters 25, 85-7

- (74. 31) A. W. Johnson and J. B. Gerardo,
"Diluent Cooling of a Vacuum-Ultraviolet High-Pressure Xenon Laser,"
J. Appl. Phys. 45, 867-72
- (74. 32) W. H. Weihofen,
"Spontaneous Decay of the "³Σ_u⁺" State of Xe₂,"
J. Chem. Phys. 60, 445-53
- (74. 33) M. C. Castex and N. Damany,
"High Resolution Spectrum of Xe₂ in the Vacuum Ultraviolet Region.
Molecular Systems Related to the Two Lower Resonance Lines,"
Chem. Phys. Letters 24, 437-40
- (74. 34) A. G. Molchanov and Yu. M. Popov,
"On the Feasibility of Electroionizational Excitation of the Vacuum
Ultraviolet Generation of Compressed Xenon,"
Kvant. Elekt. 1, 1122-8
- (74. 35) C. W. Werner, E. V. George, P. W. Hoff, and C. K. Rhodes,
"Dynamic Model of High-Pressure Rare-Gas Excimer Lasers,"
Appl. Phys. Letters 25, 235-8
- (74. 36) D. J. Bradley, D. R. Hull, M. H. R. Hutchinson, and M. W. McGeoch,
"Megawatt VUV Xenon Laser Employing Coaxial Electron-Beam
Excitation,"
Optics Comm. 11, 335-8
- (74. 37) S. C. Wallace and R. W. Dreyfus,
"Continuously Tunable Xenon Laser at 1720Å,"
Appl. Phys. Letters 25, 498-500

Y₂Spectroscopic Constants

Dissociation energy = 1.62 ± 0.22 eV, 37.3 kcal/mole, 13050 cm^{-1} .

BIBLIOGRAPHY

- (69. 1) K. A. Gingerich,
"Gaseous Metal Borides. I. On the Dissociation Energy of the
Molecules ThB, ThP, and Th₂, and Predicted Dissociation Energies
of Selected Diatomic Transition-Metal Borides,"
High Temp. Sci. 1, 258-67

Yb₂Methods of Production and Experimental Technique

Knudsen cell effusion.

Spectroscopic Constants

Dissociation energy = 4 ± 4 eV, 92 kcal/mole, 32000 cm^{-1} (72.3).

Yb₂

BIBLIOGRAPHY

- (71. 1) S. Lin and A. Kant,
"Dissociation Energies of Diatomic Rare Earth Molecules Dy₂, Ho₂,
Er₂, Tm₂, and Yb₂,"
Army Materials and Mechanics Research Center, TR No. 71-34
- (72. 2) A. Kant and S. Lin,
"Dissociation Energies of Homonuclear Diatomic Molecules of the
Rare Earths,"
Monatshefte für Chemie 103, 757-63
- (72. 3) M. Guido and G. Balducci,
"Dissociation Energy of Yb₂,"
J. Chem. Phys. 57, 5611-2

Methods of Production and Experimental Technique

Absorption.

Emission (Tesla coil, hollow cathode).

Fluorescence.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Maximum (λ) in Emission	Remarks	Bibliography
	I		Emission	5350-3890		4450	Continuum	(31.6, 31.5)
	II		Emission	3893-3776		3787	Continuum	(31.6, 31.5)
	III		Emission Absorption	3763-2936		3688	Continuum	(31.6, 31.5, 29.2)
	IV		Absorption Emission Fluores- cence	3073-2002		2550	Continuum	(31.6, 31.5, 31.4, 29.2)

Molecule Zn₂

Zn₂

III. 3763-2936Å System

Emission

In emission maximum is at $\lambda = 3688\text{\AA}$ (31.6, 31.5) and line broadens at 3076Å (31.6, 31.5).

Bands superimposed λ | 3749 | 3724 | 3706 | 3688 | 3575 | 3522 | 3483 |
3454 | 3431 | 3411 | 3052 |

Absorption

In absorption bands are without structure and maxima is at $\sim 3050\text{\AA}$ (31.6, 29.2).

IV. 3073-2002Å System

Emission (31.6, 31.5)

In emission continuous bands are 2826-2035Å, maximum is at 2550Å, line broadens at 2139Å, and diffuse bands are at $\lambda \sim 2002\text{\AA}$.

Absorption (31.6, 29.2)

In absorption continuous bands are at 2550-2002Å, maxima are at $\lambda = 2139, 2064, \text{ and } 2002\text{\AA}$, and the line broadens at 2139Å.

Fluorescence (31.3)

Numerous bands in the region 3073-2456Å.

Spectroscopic Constants

Dissociation energy = 0.25 eV(?), 6 kcal/mole(/), 2100 cm^{-1} .

BIBLIOGRAPHY

- (29. 1) Ultraviolet Absorption,
J. G. Winans,
Philos. Mag. 7, 555-66
- (29. 2) Ultraviolet Absorption,
J. M. Walter and S. Barratt,
Proc. Roy. Soc. A 122, 201-10
- (31. 3) Fluorescence,
W. Kapuscinski,
C. R. Soc. Polon. Phys. 5, 401-8
- (31. 4) Emission,
H. Hamada,
Nature 127, 555
- (31. 5) Ultraviolet and Visible Emission,
H. Hamada,
Philos. Mag. 12, 50-67
- (31. 6) Absorption and Emission, 2139, 2064, 2002Å,
J. G. Winans,
Phys. Rev. 37, 902
- (33. 7) R. Siksna,
Acta Phys. Polon. 2, 253-65
- (35. 8) Van der Waals Molecular Theory,
W. Finkelburg,
Z. Physik 96, 699-713